

Annual Meeting

September 27th-29th, 2016

Faculty of Physics, University of Vienna
Stefan Meyer Institute, Austrian Academy of Sciences

AUSTRIAN PHYSICAL SOCIETY



CONFERENCE BOOK

ACKNOWLEDGMENT

The organizers would like to thank the Faculty of Physics of the University of Vienna as well as the Stefan Meyer Institute of the Austrian Academy of Sciences for hosting the meeting. We also gratefully acknowledge our sponsors and exhibitors for their support of the conference.



Goodfellow



66TH YEARLY MEETING OF THE AUSTRIAN PHYSICAL SOCIETY

SEPTEMBER 27TH-29TH, 2016

FACULTY OF PHYSICS, UNIVERSITY OF VIENNA
STEFAN MEYER INSTITUTE, AUSTRIAN ACADEMY OF SCIENCES

ORGANISERS: CHRISTOPH DELLAGO AND EBERHARD WIDMANN

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INFORMATION

GENERAL INFORMATION

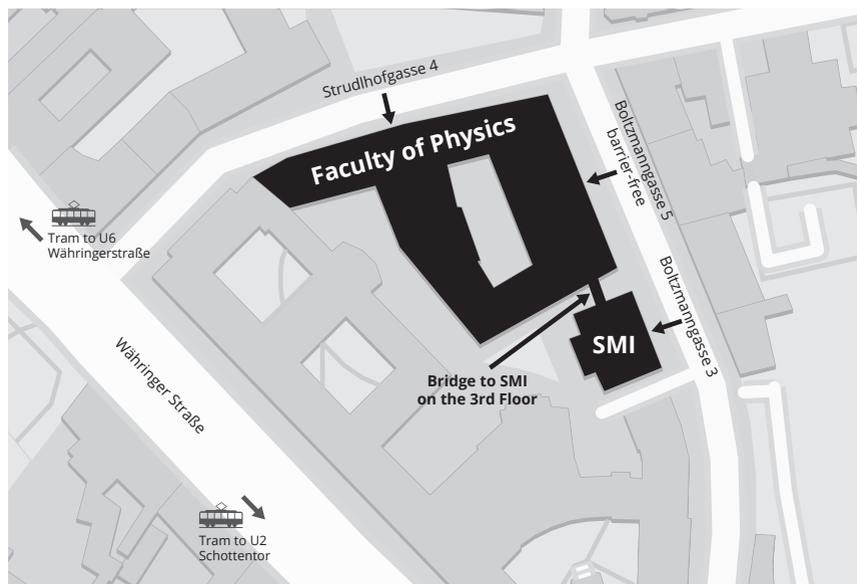
CONFERENCE WEBSITE AND REGISTRATION

<http://oepg2016.univie.ac.at/>

LOCATION

The conference will take place at the

- **Faculty of Physics** of the University of Vienna
Boltzmanngasse 5, 1090 Vienna (with access for disabled visitors),
main entrance from Strudlhofgasse 4, 1090 Vienna
- and the **Stefan Meyer Institute (SMI)** of Subatomic Physics
Austrian Academy of Sciences
Boltzmanngasse 3, 1090 Vienna



REGISTRATION/INFORMATION DESK

The registration desk is situated at the ground floor, room 3E51.

Monday	13:00 - 16:00
Tuesday	08:00 - 12:00 and 13:00 - 16:00
Wednesday	08:00 - 12:00 and 13:00 - 16:00
Thursday	08:00 - 12:00 and 13:00 - 16:00

Please report at the registration desk before attending your first session. You will receive your name badge, conference program, further documents and you can pay the conference fee.

Important: Without badge, entry to the lecture rooms will be refused.

PAYMENT

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

Payment details are shown during the online registration process. At the registration desk you can only pay cash (EUR). We do not accept credit cards.

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

CONFERENCE FEES

Members	100,- €
Non-members	130,- €
PhD student members	80,- €
PhD student non-members	100,- €
Students before master	60,- €
Day ticket	70,- €
Day ticket for teachers	40,- €

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

INTERNET

During the conference WLAN access is available for all participants via the EDUROAM network. Login data will be received with registration.

HOTELS AND ARRIVAL

All information can be found on the conference website:

<http://oepg2016.univie.ac.at/accommodation/>

PUBLIC TRANSPORT IN VIENNA

Tickets are valid for all means of transport within Vienna (Zone 100), like underground, tram, bus, and train.

They are available at the Vienna Transport Authority's ticket offices (at main stations of the underground), at ticket vending machines (at all underground stations). Many tickets are also available at tobacconists. Single tickets can be bought at vending machines inside the tram and from bus drivers. Most tickets (except weekly and monthly ticket) have to be stamped in the blue punching boxes before boarding the underground or inside trams and busses to validate them. Further information is available at www.wienerlinien.at

TICKETS	PRICE IN €
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Single Trip Ticket	2,20
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Single Trip Ticket bought on tram or bus	2,30
---	------

Wiener Einkaufskarte/Vienna Shopping Card	6,10
--	------

(valid for one day (MO – SA) from 8.00 – 20.00 h)

24 Hour Ticket	7,60
-----------------------	------

48 Hour Ticket	13,30
-----------------------	-------

72 Hour Ticket	16,50
-----------------------	-------

(valid for exactly 24, 48, or 72 hours from the time they are validated)

Vienna Card

valid for 48 hours from punching or	21,90
-------------------------------------	-------

valid for 72 hours from punching	24,90
----------------------------------	-------

(with additional discounts and benefits in shops, restaurants, and museums)

COFFEE BREAKS

The coffee breaks will take place in the Ernst-Mach-Hörsaal on the second floor of the Faculty of Physics. The conference fee covers coffee breaks and the refreshments during the poster sessions.

CONFERENCE DINNER

The conference dinner will take place on Wednesday, 28.09.2016 at 19:30. The fee is EUR 55 per person (meal and drinks). Accompanying persons are welcome. Please register in advance so we can plan accordingly. Registration for the conference dinner on site is not possible.

Heuriger „Alter Bach-Hengl“

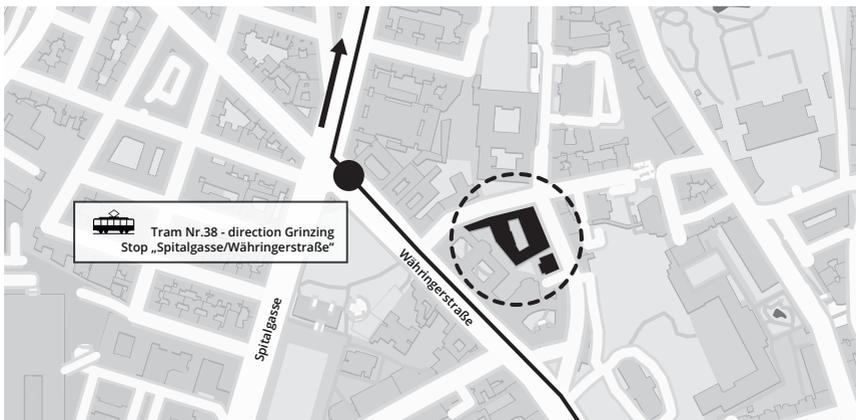
Sandgasse 7-9, 1190 Wien – Grinzing

T: +43 1 3202439

<http://www.bach-hengl.at/>

You can get from the conference site to the dinner by tram. Take tram Nr. 38 from stop Spitalgasse/Währingerstraße in direction Grinzing. Exit at the last stop called „Grinzing“ and walk approximately 4 minutes to Sandgasse 7-9 as indicated in the maps below.

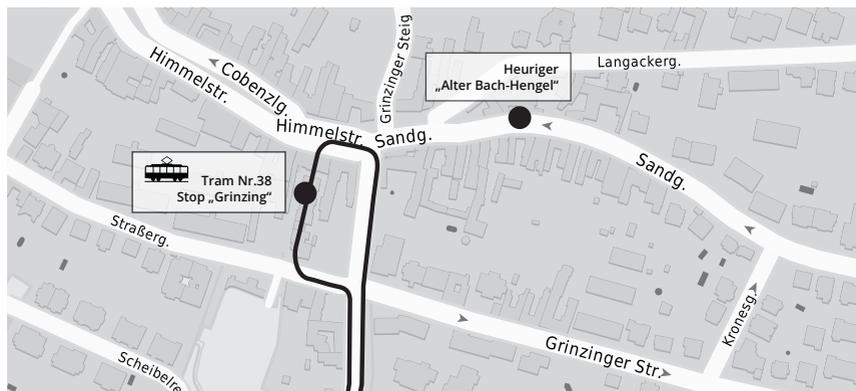
Stop „Spitalgasse/Währingerstraße“



INFORMATION

GENERAL INFORMATION

Stop „Grinzing“



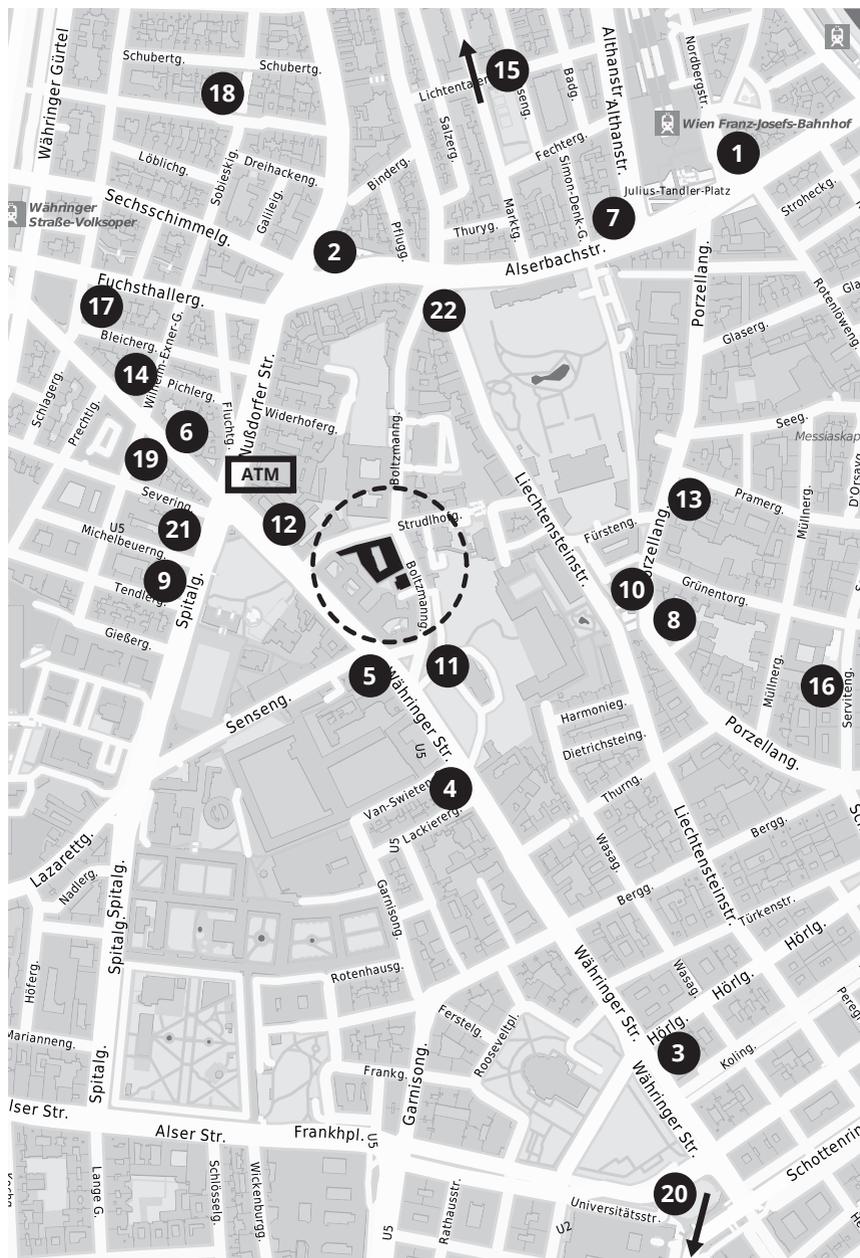
NEARBY RESTAURANTS

The restaurants near the conference site are at your disposal for lunch.

Nr.	Restaurant	Address	Web Address
1	Akakiko (Japanese)	Julius-Tandler-Platz 4	www.akakiko.at
2	Blueorange (Bagels)	Alserbachstrasse 1	www.blueorange.co.at
3	Café Francais (French)	Währinger Strasse 6-8	www.cafefrancais.at
4	Culinarium Cooking (Asian)	Währinger Strasse 21	Tel. 942 24 89
5	Masta George (Burger)	Währinger Straße 33-35	www.Masta-george.com
6	Francesco (Italian)	Währinger Strasse 66	www.ristorante-francesco.com
7	Gabel&Co (Internat., Mediterranean)	Julius-Tandler-Platz 1	www.gabelco.at
8	Gasthaus Wickerl (Viennese)	Porzellangasse 24a	www.wickerl.at
9	Giuliano 2 (Italian)	Tendlergasse 3	www.pizzeria-giuliana.at
10	Goldener Drache (Chinese)	Porzellangasse 33	www.goldener-drachen.at
11	Flein (International)	Boltzmannngasse 2	Tel. 3197689
12	Meksan (Oriental, Turkish)	Währinger Strasse 52	Tel. 276 07 88 Take-away
13	Rembetiko (Greek)	Porzellangasse 38	www.rembetiko.at
14	Café Restaurant Weimar (Viennese)	Währinger Strasse 68	www.cafeweimar.at
15	Zum Reznicek (Viennese)	Reznicekgasse 10	www.zumreznicek.at
16	Servitenwirt (Viennese)	Servitengasse 7	www.servitenwirt.at
17	Modern Korean (Korean)	Lustkandlgasse 4	http://modernkorean.at
18	The Highlander (Viennese, Pub)	Sobieskiplatz 4	www.the-highlander.at
19	VegiRant (Vegetarian/Vegan)	Wilhelm Exnergasse 16	www.vegirant.at
20	Yamm! (Vegetarian/Vegan)	Universitätsring 10	www.yamm.at
21	Noel's Food Pharmacy (Internat.)	Spitalgasse 31	www.noelsfoodpharmacy.at
22	Beaver Brewing Company (American)	Lichtensteinstrasse 69	www.baeverbrewing.at

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GENERAL INFORMATION



INFO

PROGRAM

ENERGY DAY

PLENARY

TUESDAY

WEDNESDAY

THURSDAY

POSTERS

ORAL AND POSTER PRESENTATIONS

ORAL PRESENTATIONS

If possible, please arrive at your session 15 minutes early to set up and introduce yourself to the Session Chair.

As we have a very tight schedule, please make sure to keep your time.

Occasionally (and unfortunately) the chair for a session may not appear, in which case we ask the first presenter to serve as chair of the session.

All rooms are equipped with projectors for computer and blackboards. Please bring your own laptop and adapter.

POSTER PRESENTATIONS

The Poster Sessions will take place in the afternoons of Tuesday, 27.09.2016 and Wednesday, 28.09.2016 on the 3rd floor in front of the Josef-Stefan-Hörsaal. Please bring your own fixing material (adhesive tape). The poster boards are numbered according to the program, so all participants will find their board easily. All posters are expected to be on display only on the assigned day, so they should be dismantled in the evening of the respective day. Posters that have not been removed in time will be removed by the organizers. Maximum poster size: A0 portrait (841 x 1149 mm).

We kindly ask the presenters to stay close to their respective posters during the poster sessions.

POSTER PRIZE

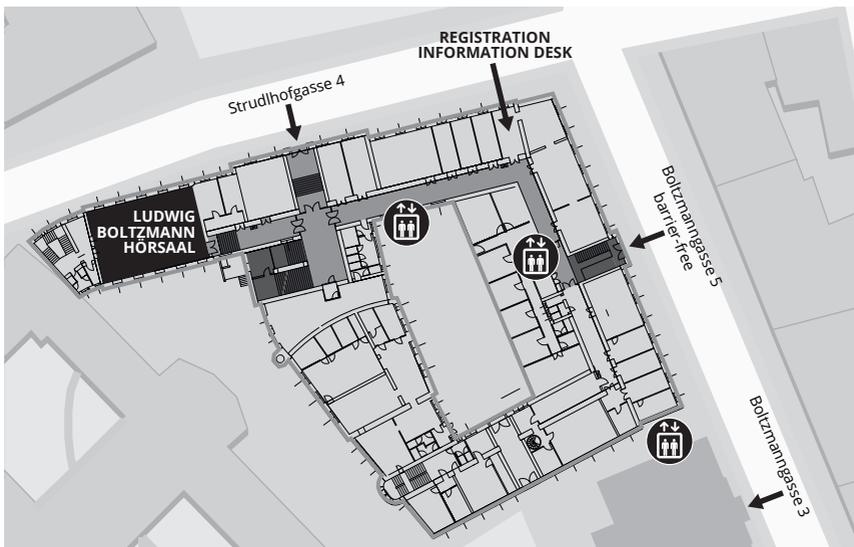
The three best posters will be awarded with poster prizes sponsored by Europhysics Letters. The winners of the poster prizes will be announced on Thursday, 29.09.2016 at 11:00 in the Lise-Meitner-Hörsaal.

TOPICS

AKU	Acoustics
AMP	Atoms, Molecules, Quantum Optics and Plasmas
COND	Condensed Matter
FAKT	Nuclear and Particle Physics
GEP	History of Physics
LHS	Physics and School
MBU	Medical Physics, Biophysics and Environmental Physics
NESY	Research with Neutron and Synchrotron Radiation
OGD	Surfaces, Interfaces and Thin Layers
PHYD	Physics for Development
PIE	Physics-Industry-Energy
STUP	Students of Physics
THEO	Theoretical and Mathematical Physics

FLOOR PLAN

GROUND FLOOR



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FLOOR PLAN

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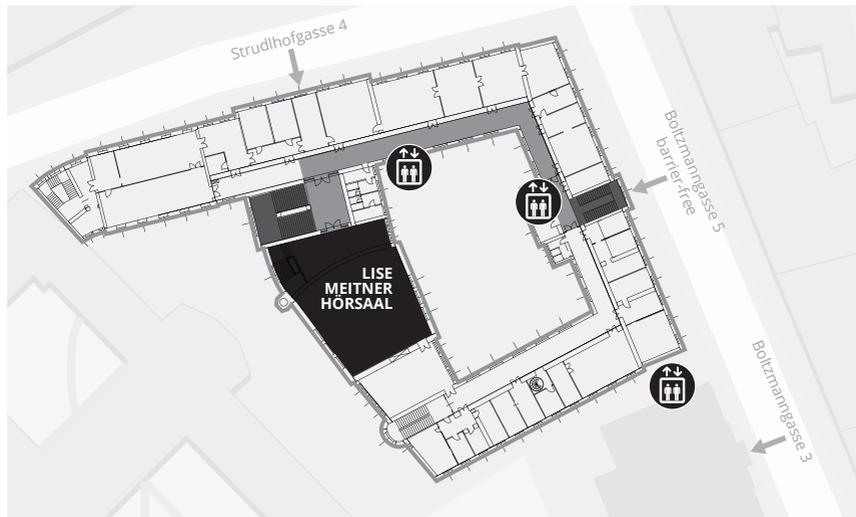
TUESDAY

WEDNESDAY

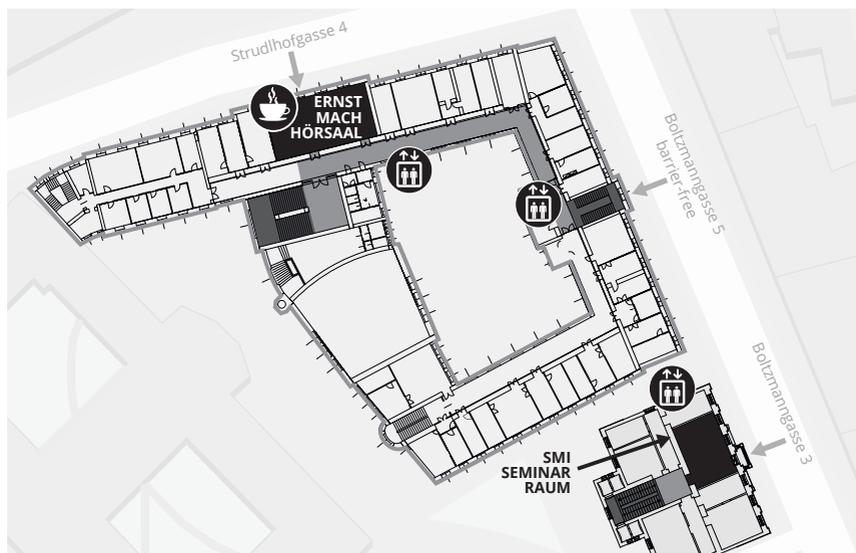
THURSDAY

POSTERS

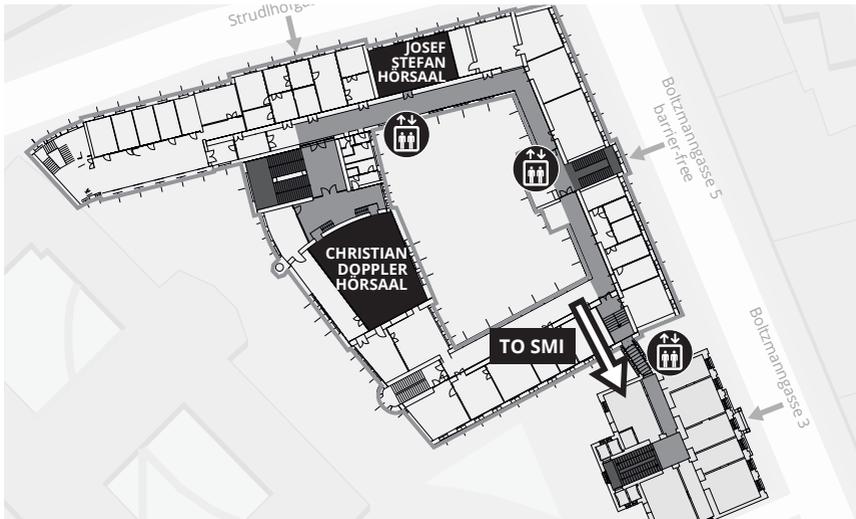
1ST FLOOR



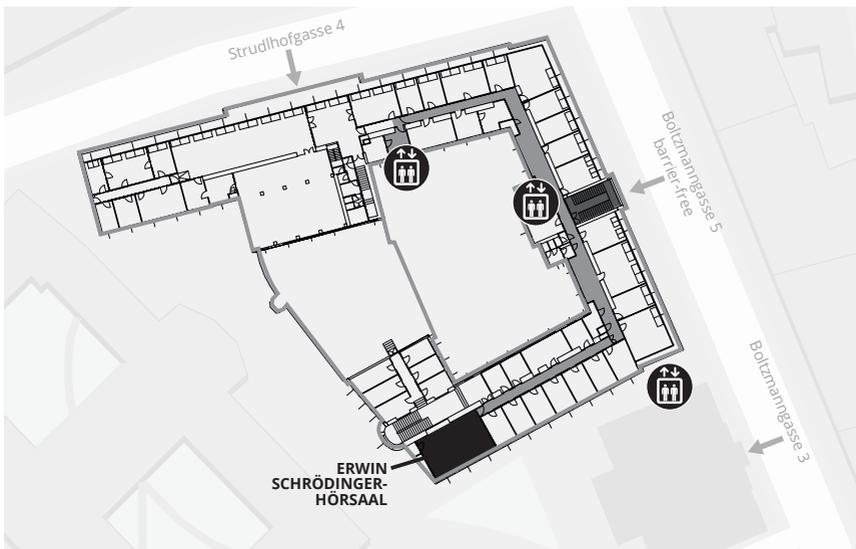
2ND FLOOR



3RD FLOOR



5TH FLOOR



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POSTERS

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VASP
www.vasp.at

PROGRAM OVERVIEW

CONFERENCE SCHEDULE

MONDAY, 26 SEPTEMBER 2016, ENERGY DAY

„Innovative Technologien für zukunftsfähige Energienetze“

Christian-Doppler-Hörsaal der Fakultät für Physik der Universität Wien,
Boltzmannngasse 5, 1090 Wien (Eingang auch Strudlhofgasse 4)

A special „Energy Day“ with focus on „Innovative technologies for sustainable energy networks“ will take place in the same venue on September 26, the day before the start of the ÖPG-Meeting. This event is independent of the main conference and will be open to the public without charge.

Energietag 2016 - „Innovative Technologien für zukunftsfähige Energienetze“ Monday, 26 September 2016 Christian-Doppler-Hörsaal der Fakultät für Physik der Universität Wien, Boltzmanngasse 5, 1090 Wien Eingang auch Strudlhofgasse 4		
Anmerkungen: .) Der Energietag ist von der Jahrestagung unabhängig und kann ohne Registrierung besucht werden. Alle Vorträge werden auf Deutsch gehalten.		
Time	ID	Energietag Moderation: Brigitte Pagana-Hammer, Werner Spitzl
10:00		Eröffnung : Brigitte Pagana-Hammer
10:15	EN1	Integration der Erneuerbaren – Harmonisierung der Beiträge zu Systemdienstleistungen im europäischen Verbundsystem, Wolfgang Gawlik (TU Wien)
11:00	EN2	Lastverteiler in innovativen Energienetzen, Klaus Hebenstreit (Verbund Trading GmbH)
11:45	EN3	Hochspannungsgleichstromübertragung (HGÜ) – eine Schlüsseltechnologie für unsere Stromversorgung, Jörg Dorn (Siemens AG)
12:30		Mittagspause
13:45	EN4	Smart Grids – die Spielwiese der Energiewende, Wolfgang Hribernik (AIT)
14:30	EN5	Urbane Netze von Morgen, Dominik Bothe & Thomas Kaufmann (TU Wien) Johannes Vavra & Thomas Karl Schuster (Wiener Netze GmbH)
15:30		Kaffeepause
16:00	EN6	Drahtlose Energieübertragung: Stand der Forschung, Applikationen, Trends Andreas Berger (Infineon)
16:45	EN7	Energiewende und Versorgungssicherheit - Ein Widerspruch?“ Franz Hofbauer (Austrian Power Grid AG)
17:30		Aperitif
18:00	EN8	<i>Abendveranstaltung:</i> Das europäische Verbundsystem zwischen Realität und Utopie, Heinrich Stigler (TU Graz)
19:30		Ende

PROGRAM OVERVIEW

TUESDAY

TUESDAY, 27 SEPTEMBER 2016

Time	Ernst-Mach-Hörsaal	Ludwig-Boltzmann-Hörsaal	Lise-Meitner-Hörsaal	Christian-Doppler-Hörsaal	
8:45	Exhibition		Official Opening		
9:00			P1 Ernst K.-H.		
9:15					
9:30					
9:45				P2 Belyaev I.	
10:00			Coffee Break Ernst-Mach-Hörsaal		
10:15			2nd floor		
10:30					
10:45					
11:00				Prize Award Ceremony	
11:15					
11:30				Fritz Kohlrusch Prize	
11:45				TUE01 Trotta R.	
12:00			Lunch Break		
12:15					
12:30					
12:45					
13:00					
13:15					
13:30					
13:45		COND/NESY	FAKT	LHS	
14:00		TUE02 Ronti M.	TUE12 Spanring M.	Roman Ulrich Sextl Prize	
14:15		TUE03 Jungblut S.	TUE13 Pree E.	TUE24 Schmid P.	
14:30		TUE04 Ramberger B.	TUE14 Spitzbart D.	Roman Ulrich Sextl Prize	
14:45				TUE25 Bodingbauer L.	
15:00		TUE05 Tröster A.	TUE15 Brandstetter J.		
15:15			TUE16 Madlener T.	VVA Laureates	
15:30			TUE17 Raucheegger C.		
15:45					
16:00					
16:15					
16:30					
16:45					
17:00					
17:15					
17:30				TUE28 Winkler A.	
17:45					
18:00					
18:15					
18:30					
18:45					
19:00					
19:15					
19:30					
19:45					
20:00					

P4 Husa S.
Evening Talk
Lise-Meitner-Hörsaal

PROGRAM OVERVIEW

TUESDAY

Time	Josef-Stefan-Hörsaal	Erwin-Schrödinger-Hörsaal	SMI Seminarraum
8:45			
9:00			
9:15			
9:30			
9:45			
10:00			
10:15			
10:30	Coffee Break Ernst-Mach-Hörsaal		
10:45	2nd floor		
11:00			
11:15			
11:30			
11:45			
12:00			
12:15	Lunch Break		
12:30			
12:45			
13:00			
13:15			
13:30			
	OGD	THEO	AMP
13:45	TUE29 Parkinson G.	TUE39 Allard Guérin P.	TUE51 Lahiri M.
14:00		TUE40 Castro Ruiz E.	TUE52 Minniberger S.
14:15	TUE30 Bliem R.	TUE41 Giacomini F.	TUE53 Tajik M.
14:30	TUE31 Müllegger S.	TUE42 Sauerwein D.	TUE54 Kauten T.
14:45	TUE32 Nacci C.	TUE43 Salzer J.	TUE55 Scheucher M.
15:00	TUE33 Jacobson P.	TUE44 Prohazka S.	TUE56 Trupke M.
15:15	Coffee Break Ernst-Mach-Hörsaal		
15:30	2nd floor		
	OGD	AKU	AMP
15:45		TUE45 Mocnik K.	TUE57 Bonneau M.
16:00	TUE34 Schmidt T.	TUE46 Wimberger P.	TUE58 Rauer B.
16:15	TUE35 Riva M.	TUE47 Reichl C.	TUE59 Wiczorek W.
16:30	TUE36 Lackner P.	TUE48 Schmiedbauer N.	TUE60 Pototschnig J. V.
16:45	TUE37 Doudin N.	TUE49 Ziegelwanger H.	TUE61 Astner T.
17:00		TUE50 Waubke H.	TUE62 Fesel J.
17:15	Poster Session 3rd floor, in front of Josef-Stefan-Hörsaal		
17:30			
17:45			
18:00			
18:15			
18:30			
18:45			
19:00			
19:15			
19:30			
19:45			
20:00			

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PROGRAM OVERVIEW

WEDNESDAY

WEDNESDAY, 28 SEPTEMBER 2016

Time	Ernst-Mach-Hörsaal	Ludwig-Boltzmann-Hörsaal	Lise-Meitner-Hörsaal	Christian-Doppler-Hörsaal	
9:00	Exhibition				
9:15			P5 Molenkamp L.		
9:30					
9:45					
10:00				P6 Sciortino F.	
10:15					
10:30			Coffee Break Ernst-Mach-Hörsaal		
10:45			2nd floor		
11:00				Fritz Kohlrausch Prize	
11:15				WED00 Monz T.	
11:30					
11:45				ÖPG Plenary Assembly	
12:00					
12:15					
12:30					
12:45					
13:00			Lunch Break		
13:15					
13:30					
			COND/NESY	FAKT	THEO
13:45		WED01 Groiss H.	WED10 Awadein M.	WED22 Merbis W.	
14:00			WED11 Jeitler M.	WED23 Schöller F.	
14:15		WED02 Klepp J.	WED12 Grossmann J.	WED24 Fajman D.M.	
14:30			WED13 Rohling H.	WED25 Steinbauer R.	
14:45		WED03 Lechner R. T.	WED14 Pitters F.	WED26 Sämann C.	
15:00			WED15 Chirita Mihaila M.C.	WED27 Gressel H.	
15:15					
15:30		Coffee Break Ernst-Mach-Hörsaal			
		2nd floor			
		COND/NESY	FAKT	THEO	
15:45		WED04 Bertel E.	WED16 Turkoglu C.	WED28 Aikens E.	
16:00		WED05 Oswald J.	WED17 Pitschmann M.	WED29 Löschner M.	
16:15		WED06 Adhikari R.	WED18 Husa S.	WED30 Sanchis-Alepuz H.	
16:30		WED07 Setman D.	WED19 Semmelrock L.	WED31 Paris-López J.	
16:45		WED08 Czibula C.	WED20 Malbrunot C.	WED32 Hebenstreit M.	
17:00		WED09 Bazarenko A.	WED21 Pradler J.	WED33 Chrusciel P.	
17:15					
17:30					
17:45					
18:00		Poster Session			
18:15		3rd floor, in front of Josef-Stefan-Hörsaal			
18:30					
18:45					
19:00					
19:15					
19:30					
19:45					
20:00		Conference Dinner			
20:15					
20:30					

PROGRAM OVERVIEW

WEDNESDAY

Time	Josef-Stefan-Hörsaal	Erwin-Schrödinger-Hörsaal	SMI Seminarraum
9:00			
9:15			
9:30			
9:45			
10:00			
10:15			
10:30	Coffee Break Ernst-Mach-Hörsaal		
10:45	2nd floor		
11:00			
11:15			
11:30			
11:45			
12:00			
12:15			
12:30	Lunch Break		
12:45			
13:00			
13:15			
13:30			
	OGD	PHYD	AMP
13:45	WED34 Franchini C.	WED44 Niemela J.	WED52 Seres E.
14:00			WED53 Goulart M.
14:15	WED35 Setvin M.	WED45 Capone B.	WED54 Lackner F.
14:30	WED36 Wagner M.		WED55 Seres J.
14:45	WED37 Hollerer M.	WED46 Cardelli C.	WED56 Winkler G.
15:00	WED38 Ghanbari E.		WED57 Meyer R.
15:15	Coffee Break Ernst-Mach-Hörsaal		
15:30	2nd floor		
	OGD	PIE (CIP)	AMP
15:45	WED39 Navarro Quezada A.	WED47 Strauss G.	WED58 Hochrainer A.
16:00	WED40 Matkovic A.	WED48 Korczak P.	WED59 Rubino G.
16:15	WED41 Kaufmann B.	WED49 Hartmann O. N.	WED60 Procopio L.
16:30	WED42 Coclite A. M.	WED50 Sevcsik E.	WED61 Ji S.
16:45		WED51 Reiter R.	WED62 Röhnsner M.-C.
17:00	WED43 Ganser C.		WED63 Mairhofer L.
17:15	Poster Session 3rd floor, in front of Josef-Stefan-Hörsaal		
17:30			
17:45			
18:00			
18:15			
18:30			
18:45			
19:00			
19:15			
19:30	Conference Dinner		
19:45			
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THURSDAY, 29 SEPTEMBER 2016

Time	Ernst-Mach-Hörsaal	Ludwig-Boltzmann-Hörsaal	Lise-Meitner-Hörsaal	Christian-Doppler-Hörsaal	
9:00	Exhibition				
9:15			P6 Hof B.		
9:30					
9:45					
10:00				P7 Salditt T.	
10:15					
10:30			Coffee Break Ernst-Mach-Hörsaal		
10:45			2nd floor		
11:00				Victor Franz Hess Prize THU01 Riegler M.	
11:15				Max Auwärter Prize THU02 Lechner B. A. J.	
11:30				Anton Paar Prize THU03 Pospischil A.	
11:45					
12:00					
12:15					
12:30					
12:45					
13:00			Lunch Break		
13:15					
13:30					
			COND/NESY	FAKT	MBU
13:45			THU04 Holzbauer M.	THU16 Spitzer H.	THU28 Leitgeb R.
14:00			THU05 Bokdam M.	THU17 Mäckel V.	
14:15			THU06 Meisels R.	THU18 Grabmayr P.	THU29 Nerattini F.
14:30			THU07 Kysylychyn D.	THU19 Jericha E.	THU30 Bianco V.
14:45			THU08 Hinkov B.	THU20 Arguedas Cuendis S.	THU31 Eicher B.
15:00			THU09 Hummer K.	THU21 Wiesinger M.	THU32 Pitters J.
15:15					
15:30		Coffee Break Ernst-Mach-Hörsaal			
		2nd floor			
		COND/NESY	FAKT	MBU	
15:45		THU10 Cardelli C.	THU22 Breibeck F. A.	THU33 Dameto de Espana M.	
16:00		THU11 Locatelli E.	THU23 Berger M.	THU34 Bauer P.	
16:15		THU12 Shabbir H.	THU24 Bulla L.	THU35 Prochazka K.	
16:30		THU13 Hartmann M.	THU25 Steinschaden D.		
16:45		THU14 Fedi F.	THU26 Zarucki M.	Open Discussion	
17:00		THU15 Domanov O.	THU27 Gosch L.		

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10:00			
10:15			
10:30	Coffee Break Ernst-Mach-Hörsaal		
10:45	2nd floor		
11:00			
11:15			
11:30			
11:45			
12:00			
12:15			
12:30	Lunch Break		
12:45			
13:00			
13:15			
13:30			
	OGD	GEP	AMP
13:45	THU36 Lechner B. A. J.	THU48 Kutschera W.	THU52 Fruehwirth S.
14:00	THU37 Hulva J.		THU53 Millen J.
14:15	THU38 Meier M.	THU49 Sachslehner F.	THU54 Brand C.
14:30	THU39 Pomp S.		THU55 Krenn M.
14:45	THU40 Mertens S. F. L.	THU50 Denoth A.	THU56 Skoff S. M.
15:00	THU41 Bayer B.		THU57 Koch M.
15:15	Coffee Break Ernst-Mach-Hörsaal		
15:30	2nd floor		
	OGD	GEP	AMP
15:45	THU42 Ruckhofer A.		THU58 Erhard M.
16:00	THU43 Tamtögl A.	THU51 Stadler L.	THU59 Handsteiner J.
16:15	THU44 Gloss J.		THU60 Pressl B.
16:30	THU45 Lasserus M.		THU61 Riahi N.
16:45	THU46 Schnedlitz M.		THU62 Mezinska S.
17:00	THU47 Balajka J.		

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MONDAY, 26.09.2016

CHRISTIAN-DOPPLER-HÖRSAAL

A special „Energy Day“ with focus on „Innovative technologies for sustainable energy networks“ will take place in the same venue on September 26, the day before the start of the ÖPG-Meeting. This event is independent of the main conference and will be open to the public without charge.

Anmerkungen:

Der Energietag ist von der Jahrestagung unabhängig und kann ohne Registrierung besucht werden. Alle Vorträge werden auf Deutsch gehalten.

Eröffnung

10:00-10:15

Brigitte Pagana-Hammer

EN1

10:15-11:00

Integration der Erneuerbaren – Harmonisierung der Beiträge zu Systemdienstleistungen im europäischen Verbundsystem

Gawlik Wolfgang

TU Wien, Institut für Energiesysteme und Elektrische Antriebe, Wien, AUT

Mit einem zunehmenden Anteil an Erzeugung elektrischer Energie aus Anlagen, die regenerative Energieträger nutzen und häufig dezentral ans europäische Verbundsystem angebunden sind, steigen auch die Anforderungen, die an diese Anlagen zu stellen sind. Während es anfangs noch ausreichend war, Störungen des Netzbetriebs durch solche

Anlagen auszuschließen, mussten sie in der Vergangenheit wenigstens netzverträglich und zunehmend systemverträglich betrieben werden. Zukünftig müssen solche Anlagen systembildend wirken können. Das bedeutet, dass sie sich im gleichen Maße, wie sie zur Bereitstellung elektrischer Energie beitragen, auch an den für den Systembetrieb notwendigen Systemdienstleistungen (Frequenzhaltung, Spannungshaltung, Netzbetriebsführung, Versorgungswiederaufbau) beteiligen können müssen.

Der Vortrag thematisiert diese Anforderungen beispielhaft an der Bereitstellung von Momentanreserve und gibt einen Überblick über deren Bedeutung und mögliche Wege, wie der Bedarf für einen stabilen Systembetrieb fair verteilt werden kann.

EN2**11:00-11:45****Lastverteiler in innovativen Energienetzen**Klaus Hebenstreit*Verbund Trading GmbH, Wien, AUT*

Der Hauptlastverteiler des Verbund ist die Schnittstelle zwischen Physik, also den Kraftwerken und ihrer Erzeugung, und dem Markt. Rund um die Uhr wird von hier der kurzfristige Einsatz der VERBUND-Kraftwerke geplant, optimiert und gesteuert sowie die Bewirtschaftung (Auf- bzw. Abstau) der Speicherseen durchgeführt.

Der Regen fällt vom Himmel, der Wind weht wann er will und die Sonne scheint unbeständig, ohne dass wir es beeinflussen können. Diese unumstößlichen Tatsachen sind wesentliche Treiber der Energiewende, denn ein Stromsystem auf Basis rein erneuerbarer Energien hat sich danach zu richten. Keine leichte Aufgabe für eine physikgetriebene Branche, in der Erzeugung und Verbrauch immer ausgeglichen sein müssen, wenn das Stromsystem sicher, leistbar und umweltverträglich sein soll.

Das geänderte Marktumfeld begleitet VERBUND nicht nur theoretisch, sondern sehr praktisch in der täglichen Arbeit, nicht zuletzt im Stromhandel, der sich der optimalen Vermarktung der Eigenerzeugung widmet. Der stark steigende Anteil erneuerbarer Energien in Europa beeinflusst das Marktgeschehen immer stärker. Der Spotmarkt, und

besonders der kurzfristige Intraday-Handel, gewinnen immer mehr an Dynamik. Seit Beginn der Liberalisierung setzten die Expertinnen und Experten von VERBUND Marktstandards bei der Optimierung des Kraftwerkseinsatzes auf Basis von energiewirtschaftlichem und meteorologischem Know-how.

EN3

11:45-12:30

Hochspannungsgleichstromübertragung (HGÜ) – eine Schlüsseltechnologie für unsere Stromversorgung

Jörg Dorn

Siemens AG, Energy Management Division, Erlangen, GER

Der beschlossene Atomausstieg in einigen Ländern und die angestrebten Ziele in Bezug auf den Kohlendioxidausstoß haben weitreichende Konsequenzen für die elektrische Energieversorgung in Europa. Die regenerative Stromerzeugung wird künftig einen erheblichen Anteil am Energiemix ausmachen, jedoch ist diese Art der Erzeugung häufig weit entfernt von den Lastzentren. In Deutschland beispielsweise werden bereits heute große Mengen an Windenergie im Norden bzw. in der Nordsee erzeugt, große Lastzentren liegen jedoch mehrere Hundert Kilometer südlich davon. Dies erfordert einen Ausbau des Übertragungsnetzes mit innovativen Lösungen. Die Hochspannungsgleichstromübertragung (HGÜ) spielt hierbei eine wichtige Rolle, da sie eine Reihe von Vorteilen gegenüber der klassischen Wechselstromtechnik mit sich bringt und bestimmte Anforderungen erst realisierbar macht, wie z.B. Kabelübertragung über längere Distanzen. Im Vortrag werden die Vorteile der HGÜ, die zum Einsatz kommenden Halbeiter sowie die grundlegenden Funktionsweisen und typischen Leistungen der verwendeten Stromrichtertopologien vorgestellt. Anhand von aktuellen Projekten werden die Anlagenkonfigurationen und Hauptkomponenten veranschaulicht.

EN4

13:45-14:30

Smart Grids – die Spielwiese der Energiewende

Wolfgang Hribernik (1,2)

(1) Austrian Institute of Technology, Wien (2) TU Graz, Graz, AUT

In Europa ist die Energiewende bereits in vollem Gang. In der Stromversorgung spielen Wind- und Sonnenenergie eine immer wichtigere Rolle. Die fluktuierende Einspeisung dieser oft auch dezentralen Energiequellen kann zu Kapazitätsproblemen auf unterschiedlichen Netzebenen führen. Intelligente Stromnetze, so genannte „Smart Grids“, nutzen durch laufende Abstimmung zwischen Erzeugern, Verbrauchern und Speichern die Systemkapazität optimal aus und erlauben so ein intelligentes Energiemanagement. Global betrachtet geht es darum, ein Bündel von Maßnahmen zu setzen, das die wichtigsten Zielparameter für die smarten Netze erfüllt: maximale Integration erneuerbarer Energieträger, höchste Versorgungssicherheit und ein volkswirtschaftlich optimales Funktionieren der Energiemärkte.

EN5

14:30-15:30

Urbane Netze von Morgen

Dominik Bothe (1), Thomas Kaufmann (1), Johannes Vavra (2), Thomas Karl Schuster (2)

(1) TU Wien, Wien, AUT (2) Wiener Netze GmbH, Wien, AUT

Die Anforderungen an urbane Versorgungsnetze sind einer erheblichen Veränderung, unter Berücksichtigung der zukünftigen Entwicklung des Energiebedarfs, unterzogen. Die Diversifikation der Energiebereitstellung und die sich ändernde Einspeisestruktur (zentral -> dezentral) beeinflussen darüber hinaus die Betriebsweise der bestehenden Netze erheblich. Daher stehen die Flexibilisierung der Energieversorgung und die energieträgerübergreifende Netzanalyse bzw. -planung im Mittelpunkt zukünftiger Betrachtungen. Diese Aspekte werden u.a. innerhalb des Projektes URBEM behandelt, wobei der Fokus auf eine gesamtheitliche, interdisziplinäre Sichtweise gerichtet ist.

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Auf Basis von getrennt durchgeführten thermischen und elektrischen Netzberechnungen, wird unter Verwendung von speziellen Methoden zur Beschreibung energieträgerübergreifender Systeme, eine Optimierungsaufgabe (z.B. Minimierung der Betriebsmittelauslastungen, Minimierung der CO₂ Emissionen) definiert und unter Berücksichtigung der technischen Rahmenbedingungen gelöst. Die im Projekt URBEM entwickelten Szenarien für den Betrachtungszeitraum 2030 und 2050 dienen als Grundlage für die Optimierung. Die Ergebnisse der Berechnungen zeigen aktuelle Auslastungen bzw. Engpässe der Versorgungsnetze sowie optimale zukünftige Versorgungsstrukturen für Entwicklungsgebiete im urbanen Raum. Die Ergebnisdarstellung erfolgt in einer speziellen Visualisierungsumgebung, in der die Versorgungsnetze und deren Auslastungen grafisch aufbereitet sind.

EN6

16:00-16:45

Drahtlose Energieübertragung: Stand der Forschung, Applikationen, Trends

Andreas Berger (1,2)

(1) Johannes Kepler Universität Linz, Institut für Signalverarbeitung, Linz, AUT (2) Infineon Technologies Austria AG, Villach, AUT

Die Idee der drahtlosen Energieübertragung wurde Ende des 19. Jahrhunderts von Nikola Tesla begründet. Die Fortschritte der modernen Halbleitertechnologie bieten Entwicklern die Möglichkeit zu Realisierung hocheffizienter Systeme und haben heute, mehr als 100 Jahre nach Tesla, zu einer Wiederbelebung der drahtlosen Energieübertragung geführt. Die Anwendungsgebiete reichen von der Übertragung einiger Milliwatt in biomedizinischen Applikationen, über wenige Watt für das Laden von Mobiltelefonen, bis hin zu hunderten von Kilowatt im Automobilbereich. Die möglichen Übertragungsdistanzen variieren je nach verwendeter Methode zwischen einigen Zentimetern bis hin zu tausenden von Kilometern. Die physikalische Grundlage dieser Technologien bildet die Energieübertragung durch elektromagnetische Wellen. Moderne Systeme verwenden je nach Applikation Wellenlängen vom Radiowellen-, über den Mikrowellen-, bis hin in den Bereich des ultravioletten Lichts. Die Schwerpunkte der aktuellen Forschung liegen

in der Optimierung der Übertragungseffizienz, der Vergrößerung der möglichen Übertragungsdistanz zwischen Sender und Empfänger und der Verbesserung der räumlichen Bewegungsfreiheit.

Dieser Vortrag gibt einen Überblick über die verschiedenen Ansätze zur drahtlosen Energieübertragung und deren physikalische Hintergründe, die etablierten Industriestandards und den aktuellen Stand der Forschung. Zusätzlich werden die Vor- und Nachteile der einzelnen Methoden anhand von ausgewählten kommerziellen und wissenschaftlichen Applikationen verdeutlicht.

EN7**16:45-17:30****Energiewende und Versorgungssicherheit - ein Widerspruch?**Franz Hofbauer*Austrian Power Grid AG, Wien, AUT*

Klimaschutz und der Ausbau erneuerbarer Energieträger (EE) sind spätestens seit der Jahrtausendwende ein präsentes Thema. Aufgrund des klaren Bekenntnisses zum Klimaschutz in Europa und der damit verbundenen starken Förderung der EE kommt es zu bedeutenden Veränderungen in der Elektrizitätswirtschaft. Diese neuen Erzeugungsformen führen jedoch zu einer höheren Volatilität im Stromsystem. Durch den Ausbau der EE geraten zudem die konventionellen Kraftwerke unter Druck. Ihre Wirtschaftlichkeit ist gefährdet, was zu Abschaltungen und Stilllegungen führt, wodurch „gesicherte“ Erzeugungsformen wegfallen und die Eingriffsmöglichkeiten im Netzbetrieb reduziert werden.

Das Übertragungsnetz ist aufgrund seiner Altersstruktur (30% älter als 30 Jahre) nicht für die neuen Anforderungen dieses fundamentalen Wandels der Erzeugungsstruktur sowie der immer kürzer werdenden Vorlaufzeiten am Strommarkt ausgelegt. Daher kommt es vermehrt zu Engpässen und den damit verbundenen Engpassmanagement-Kosten. Eine nachhaltige Lösung wiederkehrend auftretender Engpässe kann nur durch adäquaten Netzausbau bewerkstelligt werden. Allerdings benötigt der Netzausbau in der Regel um ein Vielfaches länger als die Errichtung erneuerbarer Erzeugungseinheiten. Dazu kommt, dass energiepolitische, marktwirtschaftliche und sowie umwelt- und

klimapolitische Zielsetzungen gegenwärtig nicht aufeinander abgestimmt sind, was zu einer Erhöhung der Netzbelastung und zu einem Erreichen der physikalischen Grenzen führt. Daher ist eine umfangreiche Planung und eine gründliche Analyse der Anforderungen sowie die gesamthafte Betrachtung des Elektrizitätssystems inklusive der elektrischen Netze von enormer Wichtigkeit.

Um eine ganzheitliche Darstellung des Netzausbaubedarfs zu erlangen, wird basierend auf dem APG Masterplan, den Berechnungen im TYNDP (Ten Year Network Development Plan) sowie den Anforderungen der Netzpartner der APG Netzentwicklungsplan erstellt und definiert den Netzausbaubedarf für die nächsten zehn Jahre.

All diese Werkzeuge ermöglichen es, die zukünftigen Anforderungen an die Übertragungsstruktur frühzeitig zu erkennen. Notwendige Maßnahmen können dadurch rechtzeitig geplant und realisiert werden. Die unterschiedlichen obengenannten Zeitkomponenten werden somit angeglichen und sollen damit verhindern, dass Energiewende und Versorgungssicherheit ein Widerspruch werden.

Abendveranstaltung

EN8**18:00-19:30****Das europäische Verbundsystem zwischen Realität und Utopie**Heinrich Stigler*Institut für Elektrizitätswirtschaft und Energieinnovation, TU Graz, Graz, AUT*

Aufbauende über Erörterungen welchen Beitrag die Forschungen und Inventionen zu den Innovationen am Elektrizitätsmarkt leisten können, werden das Verbundsystem den Übertragungsnetze gegenübergestellt. Die Elektrizitätsbinnenmarktrichtlinien werden einer kritische Betrachtung unterzogen und die Frage, ob die heutige Elektrizitätsmarktorganisation langfristig tragfähig und nachhaltig ist? Der Vortrag schließt mit der Frage nach der Zweckmäßigkeit der Aufbauorganisation und Ablauforganisation der Elektrizitätsmärkte ab.

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- Ivan Belyaev, ITEP, Moscow, Russia
- Karl-Heinz Ernst, EMPA, Dübendorf, Switzerland
- Björn Hof, IST Austria, Klosterneuburg, Austria
- Laurens Molenkamp, University of Würzburg, Würzburg, Germany
- Francesco Sciortino, Sapienza University, Rome, Italy
- Tim Salditt, University of Göttingen, Göttingen, Germany
- Sascha Husa, University of the Balearic Islands, Palma, Spain

TUESDAY, 27.09.2016

LISE-MEITNER-HÖRSAAL

Opening 08:45-9:00

Official Opening

P1 9:00-9:45

Molecular chirality at surfaces: 2D crystallization, electron spin filtering, single molecule manipulation and unidirectional motors

Karl-Heinz Ernst

Nanoscale Materials Science, Empa / Department of Chemistry, University of Zurich, Zurich, SUI

Molecular recognition among chiral molecules on surfaces is of paramount importance in biomineralization, enantioselective heterogeneous catalysis, and for the separation of chiral molecules into their two mirror-image isomers (enantiomers) via crystallization or chromatography. Understanding the principles of molecular recognition in general, however, is a difficult task and calls for investigation of appropriate model systems. One popular approach is thereby studying intermolecular interactions on well-defined solid surfaces, which allows in particular the use of scanning tunneling microscopy (STM). Examples of chiral amplification via the so-called 'sergeant-and-soldiers' effect as well as manipulation of chiral adsorbates via inelastic electron tunneling will be presented. In a Pasteur-type experiment at the nanoscale, molecules that constitute a dimer are spatially separated with a molecular STM tip and their absolute handedness is determined with submolecular resolution STM. Moreover, we report spin-dependent filtering of electrons by monolayers of these helical molecules. Finally the first successful electrical current-driven, unidirectional motion of a synthetic molecule will be presented.

P2

9:45-10:30

Tetra and pentaquarks at LHCb

Ivan Belyaev

Institute for Theoretical and Experimental Physics, ITEP, Moscow, RUS

The results of the study of „exotic“ multiquark states (namely tetra- and pentaquarks) at Large Hadron Collider is to be presented. The analyses are performed using full Run-I data sample accumulated by LHCb experiment in proton-proton collision at centre-of-mass energies of 7 and 8 TeV. A huge, low-background sample of beauty hadrons allows the precise study of many exotic states both in the decays of beauty particles (namely charmonium-like states and pentaquarks with hidden charm) as well as the search of exotic particles with beauty quarks.

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LISE-MEITNER-HÖRSAAL

P3**19:15-20:15****Entdeckung der Gravitationswellen**Sascha Husa*University of the Balearic Islands, Palma, ESP*

Vor 100 Jahren wurde von Albert Einstein eine völlig neue Erklärung der für uns alltäglichen und allgegenwärtigen Schwerkraft gefunden: die Krümmung der Raumzeit. Seither hat Einsteins Theorie die Physik revolutioniert, und die Fantasie von Science Fiction Autoren angeregt. Mit der Entdeckung von Gravitationswellen im September 2015, und dem Nachweis eines zweiten starken Signals im Dezember wurde eine der letzten fundamentalen Vorhersagen der Allgemeinen Relativitätstheorie direkt beobachtet: Gravitationswellen - Vibrationen in der Raumzeit, die sich mit Lichtgeschwindigkeit ausbreiten und Information über ihre Quellen mit sich tragen. Dieser Vortrag erzählt die Geschichte der Entdeckung der Gravitationswellen, erklärt genauer was diese Wellen eigentlich sind, warum vom "Hören" der Gravitationswellen gesprochen wird, und welche neuen Erkenntnisse über Astronomie und Physik sich aus der Beobachtung von Gravitationswellen ergeben. Besondere Beachtung wird die Frage finden, wie die Quellen der von LIGO gefundenen Signale als Verschmelzung zweier schwarzer Löcher identifiziert werden konnten, und was der Beitrag Österreichischer Forscher an der Entdeckung ist.

WEDNESDAY, 28.09.2016

LISE-MEITNER-HÖRSAAL

P4

9:00-9:45

Topological Physics in HgTe-based Quantum Devices

Laurens Molenkamp

University of Würzburg, Würzburg, GER

Suitably structured HgTe is a topological insulator in both 2- (a quantum well wider than some 6.3 nm) and 3 (an epilayer grown under tensile strain) dimensions.

The material has favorable properties for quantum transport studies, i.e. a good mobility and a complete absence of bulk carriers, which allowed us to demonstrate variety of novel transport effects.

One aspect of these studies is topological superconductivity, which can be achieved by inducing superconductivity in the topological surface states of these materials. Special emphasis will be given to recent results on the ac Josephson effect. We will present data on Shapiro step behavior that is a very strong indication for the presence of a gapless Andreev mode in our Josephson junctions, both in 2- and in 3-dimensional structure. An additional and very direct evidence for the presence of a zero mode is our observation of Josephson radiation at an energy equal to half the superconducting gap.

Controlling the strain of the HgTe layers strain opens up yet another line a research. We have recently optimized MBE growth of so-called virtual substrates ((Cd,Zn) Te superlattices as a buffer on a GaAs substrate), that allow us to vary the strain from 0.4% tensile to 1.5% compressive. While tensile strain turns 3-dimensional HgTe into a narrow gap insulator, compressive strain turns the material into a topological (Weyl) semimetal, exhibiting clear signs of the Adler-Bell-Jackiw anomaly in its magnetoresistance. In quantum wells, compressive strain allows inverted energy gaps up to 60 meV.

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9:45-10:30

Collective behaviour of DNA-made nanoparticles

Francesco Sciortino

Sapienza Università di Roma, Rome, ITA

DNA oligomers can nowadays be assembled to produce a large variety of nanometric constructs, via a cascade of self-assembly processes, each one guided by the length of complementary sequences of distinct DNA strands. In the lecture I will show that it is possible to build bulk quantities of DNA-made nanoparticles that closely match idealised colloids, transferring modern in-paper and in-silico intuitions into experimental realisations. I will show how unconventional collective behaviours, recently explored theoretically and numerically, can indeed be reproduced in the lab. Specifically I will discuss: (i) how to exploit limited valence interactions to suppress phase separation[1,2], enhancing the stability of the equilibrium gel phase [3-5]; (ii) how to exploit competing interactions to generate a material that is fluid both at high and at low temperatures and a solid-like disordered open network structure in between [6-7] and (iii) how to exploit bond-swap dynamics to create an all-DNA vitrimer[8-9].

[1] E. Bianchi, J. Largo, P. Tartaglia, E. Zaccarelli, F. Sciortino Phase diagram of patchy colloids: towards empty liquids, *Phys. Rev. Lett.*97, 168301, (2006).

[2] F. Sciortino and E. Zaccarelli Reversible gels of patchy particles, *Current Opinion in Solid State and Materials Science*15, 246-253 (2011).

[3] S. Biffi, R. Cerbino, F. Bomboi E. M. Paraboschi, R. Asselta, F. Sciortino and T. Bellini, Phase behavior and critical activated dynamics of limited-valence DNA nanostars, *Proc. Nat. Acad. Science*, 110 15633-15 (2013).

[4] S. Biffi, R. Cerbino, G. Nava, F. Bomboi, F. Sciortino and T. Bellini, Equilibrium gels of low-valence DNA nanostars: a colloidal model for strong glass formers, *Soft Matter*, 11, 3132 (2015).

[5] F. Bomboi, S. Biffi, R. Cerbino, T. Bellini, F. Bordi, and F. Sciortino, Equilibrium gels of trivalent DNA-nanostars: Effect of the ionic strength on the dynamics, *Eur. Phys. J. E*38: 64 (2015).

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[6] S. Roldan-Vargas, F. Smalenburg, W. Kob and F. Sciortino, Gelling by heating Scientific Report3, 2451 (2013).

[7] S. Roldán-Vargas, F. Smalenburg, W. Kob and F. Sciortino, Phase diagram of a reentrant gel of patchy particles, J. Chem. Phys. 139, 244910 (2013) ;

[8] D. Montarnal, M. Capelot, F. Tournilhac, and L. Leibler, Silica-like malleable materials from permanent organic networks, Science 334, 965 (2011).

[9] F. Romano and F. Sciortino, Switching Bonds in a DNA Gel: An All-DNA Vitrimer, Phys. Rev. Letts. 114, 078104 (2015).

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THURSDAY, 29.09.2016

LISE-MEITNER-HÖRSAAL

P6

9:00-9:45

The universality class of the transition to turbulence

Björn Hof

IST Austria, Klosterneuburg, AUT

The transition to turbulence in simple shear flows (e.g. pipe, channel and Couette flow) has remained an open problem for over a century. Typically here turbulence arises despite the linear stability of the laminar flow and results from perturbations of finite amplitude. Turbulence at first appears in the form of localised patches (e.g. puffs, spots or stripes) which coexist with laminar flow, resulting in complicated, disordered flow patterns (spatio-temporal intermittency). Individual turbulent domains can collapse or they can proliferate and seed other patches of turbulence. The time scales on which flows evolve are extremely large and likewise are the relevant length scales. Characterizing the transition process hence requires experiments of very large aspect ratios and extremely long observation times. In detailed experiments and direct numerical simulations of Couette flow we could for the first time determine the critical exponents that characterize this transition and show that it falls into the directed percolation universality class.

P7

9:45-10:30

X-ray imaging at the nanoscale: ptychography, holography and tomography

Tim Salditt

Georg-August-Universität Göttingen, Göttingen, GER

X-rays can deeply penetrate matter and thus provide information about the functional (interior) architecture of complex samples, from biological tissues and cells to nanoscale composite materials. Until recently, however, this potential of hard x-rays in view of penetration, spatial resolution, contrast, and compatibility with environmental conditions was significantly limited by the lack in suitable x-ray optics. With the advent of highly brilliant radiation, and the development of lens-less diffractive imaging and coherent focusing, the situation has changed. We now have nano-focused coherent x-ray synchrotron beams at hand to probe nanoscale structures both in scanning and in full field imaging and tomography.

We explain how the central challenge of inverting the coherent diffraction pattern can be mastered by different reconstruction algorithms in the optical far and near-field. In particular, we present full field projection imaging at high magnification, recorded by illumination with advanced x-ray waveguide optics [1], and show how imaging and diffraction can be combined to investigate biomolecular structures within biological cells. As an example we present 3d reconstructions of aggregated nano particles in macrophages, which have penetrated lung tissue [2].

[1] M. Bartels, M. Krenkel, J. Habe, R.N. Wilke, T. Salditt, X-Ray Holographic Imaging of Hydrated Biological Cells in Solution, Phys. Rev. Lett. 114, 048103 (2015).

[2] M. Krenkel, A. Markus, M. Bartels, C. Dullin, F. Alves, T. Salditt, Phase-contrast zoom tomography reveals precise locations of macrophages in mouse lungs, Sci.Rep. 5, 09973 (2015).

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TUESDAY, 27.09.2016

**Prize Award Ceremony
Lise-Meitner-Hörsaal**

11:00-11:45

FRITZ KOHLRAUSCH PRIZE WINNER TALK

LISE-MEITNER-HÖRSAAL

TUE01

11:45-12:15

Scalable Sources of Entangled Photons based on Semiconductor Quantum Dots

Rinaldo Trotta

Institute of Semiconductor and Solid State Physics Johannes Kepler University Linz, Linz, AUT

The development of scalable sources of entangled photons will bring about a revolution in quantum communication science and technology. Among the different systems under investigation, semiconductor quantum dots (QDs), also dubbed “artificial atoms”, are arguably one of the most attractive, as they can generate indistinguishable entangled photons with high efficiency and are compatible with current photonic-integration technologies. Unlike real atoms, however, no two QDs are alike. This is a major obstacle for quantum communication applications

aiming at the distribution of entanglement among distant parties. In this talk, I will propose a possible solution to this long-standing problem. I will first introduce a novel class of semiconductor-piezo-electric devices [1, 2], in which external strain and electric fields are combined to reshape the electronic structure of any arbitrary QD [3, 4] so that single and polarization-entangled photons can be generated with unprecedented quality and speed [5, 6]. Then, I will show that dynamic control over the QD in-plane strain tensor allows the energy of the entangled photons emitted by QDs to be precisely modified [7, 8] in the spectral range in which a cloud of natural atoms behaves as a slow-light medium [9], and I will demonstrate slow-entangled photons from a single quantum emitter [10]. To conclude, I will discuss how the developed technology can be exploited to build up a quantum network made of electrically-controlled QD devices interfaced with natural atoms.

[1] R. Trotta, et al. *Adv. Mater.* 24, 2668 (2012).

[2] R. Trotta, et al., in "Engineering the atom-photon interaction" (Springer, Berlin, 2015).

[3] R. Trotta, et al. *Phys. Rev. Lett.* 109, 147401 (2012).

[4] R. Trotta, et al. *Phys. Rev. B* 88, 155312 (2013).

[5] R. Trotta, et al. *Nano Lett.* 14, 3439 (2014).

[6] J. Zhang, et al. *Nature Comm.* 6, 10067 (2015).

[7] R. Trotta, et al. *Phys. Rev. Lett.* 114, 150502 (2015).

[8] J. M. Sánchez et al., *Adv. Opt. Mat.* 4, 682 (2016).

[9] J. S. Wildmann, et al. *Phys. Rev. B* 92, 235306 (2015).

[10] R. Trotta, et al. *Nature Comm.* 7, 10375 (2016).

COND/NESY**LUDWIG-BOLTZMANN-HÖRSAAL**

TUE02

13:45-14:00**Low/temperature behavior of the dipolar hard sphere fluid**Michela Ronti (1)

Alexey O. Ivanov (2), Lorenzo Rovigatti (3), Francesco Sciortino (4), Sofia S. Kantorovich (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Ural Federal University, Ekaterinburg, RUS (3) University of Oxford, Oxford, UK (4) University of Rome Sapienza, Rome, ITA

We describe self-assembly in magnetic nanocolloids by using a dipolar hard sphere (DHS) model. A DHS consists of a point dipole embedded in the center of a hard sphere that generates long-range anisotropic interactions. At low temperature DHS particles self-assemble into complex structures, with primary structures composed by rings and chains; understanding the emerging structures of the system is fundamental for designing new magnetic fluids-based devices for technological and medical applications.

We base our theoretical approach on classical Density Functional Theory, an approach that is able to capture the density and temperature dependence of the ring-chain equilibrium. [1] In order to estimate the ability of the theory to predict (i) the cluster size distribution of rings and chains at different values of the temperature and (ii) the individual cluster partition functions, we perform grand-canonical Monte Carlo simulations. We introduce specialized Monte Carlo biased moves, which favor the breaking and reforming of bonds. The knowledge of the cluster partition functions, together with our analytical approach, allows us to calculate the free energy of systems at low-to-intermediate densities, where the clusters can be considered as weakly interacting. [2]

We confirm that for low concentrations and low temperatures, the majority of magnetic nanoparticles is aggregated in rings; for higher concentrations, low temperature clusters merge together into more

complex branched structures, characterized by junctions between chains and rings. Our results will allow us to describe the next hierarchical level of self-assembly in magnetic nanocolloids: the aggregation of basic branched clusters into complex networks.

[1] S.S. Kantorovich, A.O. Ivanov, L. Rovigatti, J.M. Tavares and F. Sciortino, Phys. Chem. Chem. Phys. 17, 16601 (2015)

[2] M. Ronti, A.O. Ivanov, L. Rovigatti, F. Sciortino and S.S. Kantorovich, in preparation

TUE03

14:00-14:15

Caveats of mean-first passage time methods applied to crystallization

Swetlana Jungblut

Faculty of Physics, University of Vienna, Vienna, AUT

On the example of the crystallization transition in an undercooled Lennard-Jones fluid, I will show that the mean first-passage time based methods may underestimate the reaction rates. Then, I will provide a reason for the discrepancies in the values for the crystallization rates obtained with mean first-passage time and transition interface path sampling methods and emphasize the importance of a good definition of the reaction coordinate when applying mean first-passage time techniques.

S. Jungblut and C. Dellago, J. Chem. Phys, 142, 064103 (2015) S. Jungblut and C. Dellago, Mol. Phys, 113, 2735 (2015)

TUE04

14:15-14:30

Calculation of first derivatives in the random phase approximation for solids

Benjamin Ramberger

Faculty of Physics, University of Vienna, Vienna, AUT

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When standard DFT functionals fail to describe electronic correlation correctly, the random phase approximation (RPA) offers a valuable remedy. It is intrinsically non-local and is therefore capable of describing van-der-Waals (vdW) interactions, which, as a matter of principle, cannot be properly described by local functionals. Since vdW interactions are ubiquitous in nature there are numerous applications for the RPA. In order to make the method competitive, it is crucial to have an efficient algorithm for the calculation of forces. Only then, the RPA can be used for simulations of elastic and vibrational properties as well as for structure relaxations. Here we present a novel method to efficiently calculate first derivatives of RPA energies in extended systems, by using the Green's function formalism from quantum many body theory in combination with the projector augmented wave (PAW) method. We also show first results from an implementation of this new method in the VASP code, including phonon spectra of graphite and diamond from a 128 atom supercell and a comparison with finite differences.

TUE05

14:30-15:00**Finite Strain Landau Theory Applied to the High Pressure Phase Transition of Lead Titanate**Andreas Tröster*Vienna University of Technology, Institute of Material Chemistry, Vienna, AUT*

The concept of broken symmetry is central to many areas in physics. In particular, Landau theory (LT) an indispensable cornerstone of the theory of structural phase transitions. On the other hand, the last decades have seen a tremendous success of ab initio methods in condensed matter physics. Yet, the concepts of DFT and LT are to some extent antipodal. Indeed, condensed matter broken symmetry phases usually appear at low temperature and are thus accessible by ab-initio methods. However, as a rule the high symmetry reference phase, which is the pivotal reference frame of LT, only exists at elevated temperatures. DFT and LT thus appear as complimentary concepts, and the question of how to blend these two approaches in an efficient way has been an active area of research for the last two decades.

In particular, DFT calculations are indispensable for understanding

high pressure phase transitions. Unfortunately, while imposing high pressure usually does not impose serious additional difficulties in DFT, an attempt to similarly extend LT to include high pressure phase transitions that involve nonlinear elasticity as a central ingredient turns out to be a non-trivial enterprise. Yet, recently we have succeeded in constructing such an extension [PRX 4, 031010 (2014)] and have demonstrated both its practical applicability as well as the tremendous increase in numerical precision over a standard Landau description by applying it to the archetypal perovskite SrTiO₃. An essential ingredient for the success of this approach is the ab initio calculation of pressure-dependent elastic constants.

The ferroelectric cubic-tetragonal phase transition in the closely related perovskite PbTiO₃, one of the most-studied ferroelectrics with considerable importance in technology, provides a striking example in which standard LT not only fails quantitatively but actually breaks down completely. This is obvious taking into account that high precision x-ray data obtained by Janolin et al [PRL 101, 237601 (2008)] at room temperature reveal a second order pressure-induced phase transition at $P_c=13\text{GPa}$, whereas the T-driven ferroelectric transition at $T_c \approx 763\text{K}$ appears to be first order. Moreover, the spontaneous strain components accompanying the high pressure transition at room temperature show a peculiar pressure-dependence with curvatures that are completely at odds with the predictions of standard LT.

In the present talk, I will demonstrate how our new flavor of DFT-aided finite strain LT combined with a quasiharmonic approximation immediately resolves these issues in a straightforward way. Our theory also holds considerable predictive power, as it offers to determine e.g. the (P,T) -dependence of elastic constants in the low symmetry phase, the pressure dependence of the soft mode frequency and the $P_c(T)$ phase boundary including the location of the tricritical point.

TUE06

15:45-16:00

Nucleation and structural growth of cluster crystals

Christian Leitold

Christoph Dellago

Faculty of Physics, University of Vienna, Vienna, AUT

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We study the nucleation of crystalline cluster phases in the generalized exponential model with exponent $n=4$. Due to the finite value of this pair potential for zero separation, at high densities the system forms cluster crystals with multiply occupied lattice sites. Here, we investigate the microscopic mechanisms that lead to the formation of cluster crystals from a supercooled liquid in the low-temperature region of the phase diagram. Using molecular dynamics and umbrella sampling, we calculate the free energy as a function of the size of the largest crystalline nucleus in the system, and compare our results with predictions from classical nucleation theory. Employing bond-order parameters based on a Voronoi tessellation to distinguish different crystal structures, we analyze the average composition of crystalline nuclei. We find that even for conditions where a multiply-occupied fcc crystal is the thermodynamically stable phase, the nucleation into bcc cluster crystals is strongly preferred. Furthermore, we study the particle mobility in the supercooled liquid and in the cluster crystal. In the cluster crystal, the motion of individual particles is captured by a simple reaction-diffusion model introduced previously to model the kinetics of hydrogen bonds.

TUE07

16:00-16:15**Pressure-Induced Bulk-Melting in Water Ice**Clemens Moritz

Christoph Dellago

Faculty of Physics, University of Vienna, Vienna, AUT

Apart from its rich phase diagram of thermodynamically stable phases, water ice can also be found in glassy phases called amorphous ices. While often produced by rapid cooling, such ices also form when ice Ih cooled to 77 K is subjected to pressures on the order of 1 GPa in a process called pressure induced amorphization (PIA) [1]. Based on experimental evidence as well as on results from molecular simulation, multiple transition mechanisms have been proposed for this process: thermal and mechanical melting, as well as a cross-over scenario between the two [2,3]. However, direct simulations suffer from an inherent bias towards mechanical melting due to the disparate timescales accessible in simulation and experiment.

We approach the subject of PIA by studying pressure-induced bulk-melting in water ice using computer simulations employing the TIP4P/Ice water model [4]. In particular, we use path-based rare-event techniques such as transition interface sampling (TIS) [5] to sample dynamical trajectories of melting events at successively lower temperatures and increased pressures in an effort to overcome the timescale problems of molecular simulation. These calculations allow us to investigate the transition mechanism by analysing the resulting trajectories, thereby elucidating the influence of increased pressure and reduced temperature on the formation of defects within the crystal structure.

- [1] O. Mishima, L.D. Calvert, and E. Whalley, *Nature* 310, 393 (1984).
- [2] T. Strässle, S. Klotz, G. Hamel, M. Koza, and H. Schober, *Phys. Rev. Lett.* 99, 175501 (2007).
- [3] J.S. Tse and D.D. Klug, *Phys. Chem. Chem. Phys.* 14, 8255 (2012).
- [4] J.L.F. Abascal, E. Sanz, R. García Fernández, and C. Vega, *J. Chem. Phys.* 122, 234511 (2005).
- [5] T.S. van Erp, D. Moroni, and P.G. Bolhuis, *J. Chem. Phys.* 118, 7762 (2003).

TUE08

16:15-16:30

Cavitation of water under tension

Georg Menzl

Christoph Dellago

Faculty of Physics, University of Vienna, Vienna, AUT

Due to its strong cohesion, liquid water can sustain tensions exceeding -120 MPa for long times before the system decays into the vapor phase via cavitation, i.e., bubble nucleation [1]. Cavitation of water under tension has implications for many biological processes, like water transport in trees or the spore propagation of ferns. Recent interest in the topic is magnified by the discrepancy between estimates for the cavitation pressure obtained via different experimental methods [2].

Due to the short time-scale on which the transition takes place and the small volume of the critical bubble at experimentally feasible conditions, direct observation of cavitation at the microscopic level remains

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elusive. Hence, computer simulations are a natural choice to investigate cavitation in water with molecular resolution on the time-scales governing the emergence of microscopic bubbles in the liquid. We investigate the structure and dynamics of vapor bubbles emerging from metastable water at negative pressures and ambient temperature. At these conditions, bubbles are essentially empty cavities in the liquid which are irregularly shaped in the early stages of cavitation and become more spherical as they grow [3]. Nevertheless, the free energy of bubble formation can be accurately reproduced in the framework of classical nucleation theory if the curvature dependence of the surface tension is taken into account. Comparison of the observed bubble dynamics to the predictions of the macroscopic Rayleigh–Plesset equation, augmented with thermal fluctuations, demonstrates that the growth of nanoscale bubbles is governed by viscous forces. Combining the dynamical prefactor determined from the Rayleigh–Plesset equation with the free energy of classical nucleation theory yields an analytical expression for the cavitation rate that reproduces the simulation results very well over a wide range of pressures.

Furthermore, our results indicate that entropy is the driving force behind bubble nucleation at ambient temperature. The bubble entropy per surface area decreases linearly with the bubble curvature which suggests a connection to broken hydrogen bonds at the bubble–liquid interface.

[1] M. El Mekki Azouzi, C. Ramboz, J.F. Lenain, F. Caupin, *Nature Physics* 9, 38 (2013)

[2] F. Caupin, E. Herbert, *Comptes Rendus Physique* 7, 1000 (2006)

[3] G. Menzl, M. A. Gonzalez, P. Geiger, F. Caupin, J. L. F. Abascal, C. Vale-riani, and C. Dellago, arXiv:1606.03392 (2016)

TUE09

16:30-16:45**Non classical freezing of hard cube colloids**Carina Karner

Christoph Dellago

Faculty of Physics, University of Vienna, Vienna, AUT

Classical nucleation theory (CNT) is the most prominent phenomenological theory to describe first order phase transitions. In CNT, spherical droplets of the new stable phase grow within the old, metastable phase via an one-step Markov process. Despite its great success in predicting nucleation rate and free energy barrier trends in a wide variety of systems, there is a growing number of phenomena that do not fit into the CNT framework and those cases are subsumed under the term “non-classical nucleation”.

In this work [1] we provide strong computational evidence that hard colloidal cubes, a system whose thermodynamic properties have been studied experimentally [2] as well as theoretically [3], crystallise via a non-classical two-step process: We observe that orientational order precedes cubic crystalline order and more specifically, that orientational order acts as template for the cubic lattice to grow on. This dominance of the orientational ordering during the transition suggests that the hard cube crystallisation bears in fact a greater resemblance to the isotropic-nematic transition in liquid crystals than to the crystallisation of conventional isotropic colloids.

Concluding, we have shown through the the use of kinetic Monte Carlo simulations that hard cube colloids, a relatively simple system, exhibits a complex freezing behaviour and we hope that this research inspires further studies of the freezing of anisotropic colloids.

[1] „Non classical freezing of hard cube colloids“, Carina Karner and Christoph Dellago, to be submitted

[2] Laura Rossi, Vishal Soni, Douglas J Ashton, David J Pine, Albert P Philipse, Paul M Chaikin, Marjolein Dijkstra, Stefano Sacanna, and William T M Irvine. Shape- sensitive crystallization in colloidal superball fluids. Proceedings of the National Academy of Sciences of the United States of America, 112 (17):5286–90, 2015.

[3] Umang Agarwal and Fernando A Escobedo. Mesophase behaviour of polyhedral particles. Nat Mater, 10 (3):230–235, 2011

TUE10

16:45-17:00**Crystallisation behavior of VHDA in the high-pressure regime**Josef Stern*University of Innsbruck, Institute of Physical Chemistry, Innsbruck, AUT*

The aim of my work is focussing on the crystallisation behavior (i.e., crystallisation temperature and kinetics) of very high-density amorphous ice (VHDA) in the higher-pressure regime. By examining the volume curves in dependence from the temperature in-situ it is possible to extract onset and offset temperatures of crystallisation. Further ex-situ powder X-ray diffraction yields information on the obtained crystalline phase/phases.

One of the peculiarities that make water such a fascinating substance to study is the abundance of solid phases it can form. Due to its polymorphic properties as many as 17 distinct crystalline phases could be described scientifically thus far, with more expected to be discovered. Also in the disordered solid state water appears to exhibit this unusual diversity: three different amorphous solid phases have been distinguished, labelled by their variation in density: low-density amorphous ice (LDA), high-density amorphous ice (HDA) and very high-density amorphous ice (VHDA). As to the true nature of these phases and their distinctness from each other there has been much debate in the past decades. Least explored of these phases, and the most recent to have been described is VHDA. This work is focussed on the examination of VHDA's crystallisation behavior in the higher pressure regime (0.70 - 1.80 GPa), with respect to its crystallisation temperature. Various heating rates have been applied to study the kinetics involved. In comparison to results formerly obtained for unannealed high-density amorphous ice (uHDA) it shows that especially at lower pressures VHDA exhibits a higher thermal stability against crystallisation as uHDA. While at higher pressures they appear to converge. Furthermore, it appears to make a difference at which pressure VHDA is produced from uHDA (1.10, 1.60 or 1.90 GPa). The higher the pressure (of formation from uHDA), the more thermally stable VHDA becomes against crystallisation when being heated isobarically at a given pressure.

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TUE11

17:00-17:15

Synthesis and characterisation of a fast Li-ion conductor

Li7-x-yLa3Zr2-x-yNbxTayO12

Maria Elisabeth Maier

Andreas Reyer, Maurizio Musso, Georg Amthauer

Paris Lodron University of Salzburg, Salzburg, AUT

Technologies for renewably generated energy and its storage in de-localised stationary systems as well as portable devices belong to the important contemporary challenges. In general, Li-ion secondary batteries are among the most promising electrical energy storage technologies. Especially all-solid-state Li-ion batteries have been extensively studied in recent years, because they have some advantages. They show high volumetric and gravimetric energy densities at high power densities, comply with safety requirements, and provide further desirable properties like thermal and mechanical stability. Garnet-like, cubic ceramics Li7-x-yLa3Zr2-x-yNbxTayO12 ($0 \leq x+y \leq 2$) (LLZNTO) are promising solid-state electrolytes [1], not least because of their good chemical stability against various electrode materials, especially Li metal. (i) All samples have garnet-like structures and belong to the garnet supergroup: at ambient conditions the endmember Li7La3Zr2O12 (LLZO) and low substituted LLZNTOs have the tetragonal structure I41/acd (henritermierite group); all of the other samples show the cubic phase Ia-3d (garnet group). (ii) Practical applications in all-solid-state batteries demand electrolytes with ionic conductivities of at least $\sigma \geq 10^{-4} \text{ S cm}^{-1}$ (so called “fast ionic conductors”). Tetragonal LLZO has a low ion conductivity of about $10^{-6} \text{ S cm}^{-1}$. Higher ionic conductivities can only be achieved via substitution and stabilisation of the cubic phase. [2] (iii) A cubic structure is a necessary, although not a sufficient, condition for high ionic conductivity in LLZNTOs. Generally speaking, the ionic conductivity is a function of the amount of charge carriers and their mobility in a compound. In cubic LLZNTOs the ionic conductivity is promoted by the following factors: (a) low substituent concentrations: low x+y just above the phase transition concentrations supply great amounts of Li-ion; (b) ceramics: dense sintered materials yield a highly disordered Li-sublattice (“liquid-like solids”) and low grain-boundary resistances. This study presents the preparation and characterisation

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of fast Li-ion conductors LLZNTOs. The samples are characterised by standard methods like XRPD and SEM (BSE, EDX). A special focus of the characterisation lies on Raman spectroscopy. [3] Polarised and non-polarised Raman measurements with different laser wavelengths at various (especially low) temperatures and with an electrically gated (100 ps) Raman equipment for suppressing fluorescence will elucidate the LLZNTO-structure and will support the determination of phases (cubic, tetragonal), phase transitions (concentration-dependent, temperature-dependent), inhomogeneities (structural, chemical), and order-disorder-phenomena (statical, dynamical).

[1] Tong X., Thangadurai V., Wachsman E.D., Inorg. Chem. 2015, 54, 3600.

[2] Thangadurai V., Pinzaru D., et al., J. Phys. Chem. Lett. 2015, 6, 292.

[3] Mukhopadhyay S., Thompson T. et al., Chem. Mater. 2015, 27, 3658.

FAKT

LISE-MEITNER-HÖRSAAL

TUE12

13:45-14:00

Measurement of Higgs and Z boson decays to a pair of tau leptons with CMS

Markus Spanring

HEPHY, Austrian Academy of Sciences, Vienna, AUT

The main irreducible background for Higgs bosons decaying to a pair of tau leptons is Z to tau tau. In this talk, the cross section measurement with 2015 data for a Z boson decaying to a pair of tau leptons is presented. The focus is on background estimation methods. Additionally, a study of Higgs boson decays to a pair of tau leptons including a first glimpse of a MVA approach for signal extraction will be shown.

TUE13

14:00-14:15

The planned High Granularity Calorimeter of the CMS experiment at the High-Luminosity LHC

Elias Pree

HEPHY, Austrian Academy of Sciences, Vienna, AUT

The Compact Muon Solenoid (CMS) is one of the biggest experiments at the Large Hadron Collider (LHC). It is a general-purpose detector and has a broad physics programme, which includes the study of the standard model, higgs boson, the search for extra dimensions and particles that could make up dark matter.

The detectors of CMS are subdivided in a multitude of different layers. One of these is the calorimeter, which is used to measure the energy of jets and particles.

Due to a future increase of luminosity by a factor of 5, current detector applications of the calorimeter endcap have to be replaced because of radiation damage. For an integrated luminosity of 3000 fb^{-1} the electromagnetic calorimetry near shower max will sustain integrated doses of 1.5 MGy and neutron fluences of 10^{16} n/cm^2 . Additionally due to the effects of the increased number of collisions the identification of different electromagnetic objects becomes more challenging.

To address these challenges, CMS will build a new high-granularity sampling calorimeter, which enables the application of particle flow methods within the calorimeter to optimize jet energy resolution.

The electromagnetic calorimeter section will consist of silicon sensors with tungsten absorbers. The front hadronic section will use brass or steel as absorber and silicon sensors as well. The back hadronic section will use plastic scintillators as active material and brass as absorber.

The talk will provide insight in the layout of the hexagonal prototype silicon sensors, which will be manufactured by commercial silicon foundries. The Development of a quality assurance scheme for both the prototype sensors in the R&D phase and during the mass production of several thousand sensors is an essential component. With that in mind a test setup was constructed to measure smaller prototype sensors. Different measurements will be presented and the results of these will be used for the identification of flaws in the measurement setup and the design of the real-sized sensors.

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TUE14

14:15-14:30**Search for supersymmetry in pp collisions at 13 TeV in the single lepton final state with the CMS experiment**Daniel Spitzbart*HEPHY, Austrian Academy of Sciences, Vienna, AUT*

Results are presented from a search for supersymmetric particles in events with final states containing a single lepton and multiple jets, none of which are identified as originating from a b quark. The data set corresponds to proton-proton collisions with an integrated luminosity of 2.3 fb^{-1} , recorded by the CMS experiment at $\sqrt{s} = 13 \text{ TeV}$. The signal model describes gluino pair production with masses in the TeV range.

The cascade decay of each gluino involves production of 1st and 2nd generation quark jets and a neutral stable supersymmetric particle, the lightest neutralino, which leads to a significant amount of missing transverse energy. The angle between the reconstructed W boson and the lepton coming from its decay is used as main discriminative variable between signal and background.

A robust method to estimate background events using control samples in data is implemented. Yields in data are found to be compatible with the expectation from standard model background processes, and exclusion limits on gluino and neutralino masses are obtained.

TUE15

14:30-14:45**Tau Identification Studies for High-Luminosity LHC Upgrade**Johannes Brandstetter*HEPHY, Austrian Academy of Sciences, Vienna, AUT*

During LHC run 2 and especially for the High-Luminosity LHC upgrade a stepwise increase of luminosity is planned. This leads to new challenges for the detectors concerning e.g. radiation exposure and pile-up. In this talk the reconstruction of hadronically decaying tau leptons at CMS is outlined and the impact on the identification of taus at CMS for

different upgrade scenarios is studied. The focus is on the required changes and reoptimization of the tau reconstruction algorithms.

TUE16

14:45-15:00

Quarkonium production and polarization in pp collisions at CMS

Thomas Madlener

HEPHY, Austrian Academy of Sciences, Vienna, AUT

Studies of quarkonium production are important to improve our understanding of hadron formation within the context of quantum chromodynamics. This talk presents CMS results on quarkonium production in pp collisions with emphasis on the most recent measurements. In particular, the cross sections of the five S-wave quarkonium states at 13 TeV will be discussed. Moreover, the newest results on P-wave quarkonia will be presented.

TUE17

15:00-15:15

Track reconstruction in the ATLAS Inner Tracker at the High Luminosity LHC

Christoph Rauchegger

Institut für Astro- und Teilchenphysik, University of Innsbruck, Innsbruck, AUT

After the High Luminosity upgrade of the Large Hadron Collider (HL-LHC) it should operate with a luminosity about ten times higher than at present, corresponding to approximately 200 inelastic pp collisions at each beam-crossing. Due to the increased luminosity and the accumulated radiation damage the current ATLAS Inner Tracker has to be replaced. Based on the experience gained with the current tracker, a new all-silicon tracker design has been developed. To search for signatures of new physics ATLAS has to perform charged particle reconstruction in the very forward region of the detector. The design changes make it necessary to revise the track reconstruction process. The performance of this process is studied using fully simulated Monte Carlo events.

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TUE18

15:45-16:00**Optimising strip-isolating structures in silicon sensors for tracking detectors**Viktoria Hinger*HEPHY, Austrian Academy of Sciences, Vienna, AUT*

N-in-p type silicon strip sensors, as they will be used in the Phase II upgrade of the CMS tracker for the High-luminosity LHC, employ a special structure of high p doping, the so-called p-stop, to separate the individual strips. If an ionising particle hits the sensor, the resulting charge is divided between the strips closest to its track. To determine the best possible layout of the sensors, the charge loss, occurring when a particle hits the strip-isolating p-stop structure, is investigated.

For these studies a new experimental setup has been commissioned at the Institute of High Energy Physics in Vienna, using the so-called ALiBa-Va readout system and an external 50 picosecond pulsed laser source to generate signals in the sensors. With this setup the detector response to minimum ionising particles is simulated, which allows to study the geometry of the electric field inside the sensor and thereby understand the role the p-stop layer plays in the charge distribution inside the sensor. First results of comparative studies with various prototype sensors will be presented and an outlook at possible sensor layouts for future tracking detectors will be made.

TUE19

16:00-16:15**Simulation of an ultrafast gamma detector with GEANT4**Florian Dachs (1)

Stefan E. K. Brunner (2), Albert Hirtl (1), Dennis R. Schaart (2), Lembit Sihver (1,3)

(1) Atominstytut, TU Wien, Vienna, AUT (2) Radiation Science and Technology, TU Delft, Delft, NED (3) EBG MedAustron, Wiener Neustadt, AUT

High time resolution is becoming increasingly important for many applications in nuclear medicine (e.g. time-of-flight positron emission

tomography), high energy and nuclear physics applications and material science (e.g. Positron Annihilation Lifetime Spectroscopy, PALS). One approach to improve the time resolution of such detectors is the application of silicon photomultipliers (SiPM) as photodetectors. Recently, a completely digital SiPM was introduced: the digital photon counter (DPC), developed by Philips.

Digital silicon photomultipliers are built from an array of single photon avalanche diodes (SPAD) which are sensitive enough to detect even single photons. They offer high gains at low voltage, a fast response, 2D resolution, are almost immune to magnetic fields and have very small dimensions which allows for very compact and robust detector designs. A new design for a gamma detector comprising several dSiPMs and a large monolithic cerium doped lutetium-yttrium oxyorthosilicate (LYSO:Ce) scintillation crystal has been simulated using the particle transport software Geant4. It provides both, high light yield and short decay time, thus making it a good choice for fast timing applications. With the modular design of Geant4 it is easy to switch between different physics models and geometries, thus allowing for an extensive study of various setups. Eventually, the goal of this simulation is to compare various physics models and detector geometries based on their performance in terms of energy and time resolution.

First results of an analysis of simulated data for the detection efficiency of 511keV photons, the probabilities of various photon interactions within the scintillator and the spatial and temporal distribution of scintillation photons impinging on the dSiPMs will be presented. Furthermore, the results obtained for several variations of the detector's geometry and for various physics models as provided by Geant4 will be discussed.

TUE20

16:15-16:30

Top quark mass calibration for Monte-Carlo event generators

Moritz Preißer (1)

Bahman Dehnadi (1), Andre Hoang (1), Vicent Mateu (2), Iain Stewart (3)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Universidad Autónoma de Madrid, Madrid, ESP (3) Massachusetts Institute of Technology, Cambridge, USA

The lack of knowledge how the top quark mass parameter in Monte-Carlo

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event generators (MCs) is related to field theoretically defined mass schemes limits the theoretical interpretation of the top quark mass measurements based on templates obtained from direct reconstruction analyses at hadron colliders. Since these measurements are the most precise which are available today, clarifying this issue is very important.

In the first part of the talk I review the conceptual aspects of the problem and argue which classes of field theoretic heavy quark mass definitions have a close relation to the quark mass parameter in MCs. In the second part I describe a method to calibrate the top quark MC mass parameter by fits of MC hadron level predictions for observables with very strong mass sensitivity to corresponding hadron level QCD predictions. I demonstrate the approach for thrust in electron positron collisions using factorization based QCD calculations at NNLL/NLO that account for hadronization and the complete top mass dependence, and I present concrete numerical results.

TUE21

16:30-16:45**The calculation of differential and double differential cross sections using GATE simulations**

Alexander Burker (1)

Albert Hirtl (2), Lembit Sihver (1,2)

(1) Atominstitut, TU Wien, Vienna, AUT (2) EBG MedAustron, Wiener Neustadt, AUT

During the last decades carbon beam therapy has become an important treatment method for treating cancer, especially for patients with deep seated and radio-resistant tumors. One established way of treatment is conventional radiation therapy using photons or electrons. However, due to its favorable depth-dose distribution, healthy tissue can be spared better when using protons or light ions. While electrons have a short range and X-rays deposit most of their energy shortly after the surface, charged particles have a dose distribution with a peak – the Bragg Peak – at a certain depth, which depends on the projectile, its kinetic energy and the target properties. Aside from the possibility to deposit the energy at a controllable depth in the tissue, charged particles transfer only little energy to the healthy tissue on their passage

through it and that way spare vulnerable organs outside the targeted tumor region.

In ion-beam therapy, ions are used instead of protons, due to their higher biological impact at the terminal depth. However, when heavy ions collide with atoms, nuclear reactions will produce lighter ions that travel further than the primary terminal depth. This contributes to a dose beyond the Bragg Peak and causes a so called fragmentation tail. Production of secondary particles is highly dependent on the total reaction cross section, which in turn, is dependent on the projectile type and energy and the target. In order to calculate the applied dose in treatment planning, knowledge of the differential and double differential cross sections is necessary. Unfortunately, there are only little experimental data available currently.

Until more data can be deduced from measurements it is possible to use Monte Carlo simulation software to estimate the desired cross sections. There are several software packages available, that can simulate particle transport and nuclear reactions, like Geant4, FLUKA and PHITS. The core of this work was to produce differential and double differential cross section estimates from Geant4 simulations of a carbon particle beam passing through a thin target. These simulations had to be repeated for several iterations of projectile energies, as well as target materials. To obtain the cross sections, an analysis program was developed, that can filter the simulation output for specific particles, based on their type, energy and location. After counting the filtered particles, the program can calculate both types of cross sections and store them on the hard disk.

Results of the comparison between simulated data and data from literature will be presented. Additionally, the influence of parameters such as target material, the angle of detection and the ejected particle type on the agreement between data and simulation will be discussed.

TUE22

16:45-17:00

Interpreting the Simplified-Model Results from the LHC with SModels

Federico Ambrogi

HEPHY, Austrian Academy of Sciences, Vienna, AUT

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We present SModelS, a tool designed for the decomposition of theories Beyond the Standard Model (BSM) into their Simplified Models Spectra (SMS).

After decomposing a generic model to its SMS, SModelS compares the theoretical predictions on the production cross sections with the results from the LHC searches, implemented in a comprehensive and up-to-date database. We present the recent developments of version 1.1, that makes use of signal Efficiency Maps (EM) for the computation of upper limits on production cross sections. By using public tools like MadAnalysis5 and CheckMATE we are able to produce efficiency maps outside the LHC collaborations and enrich our experimental database. We focus here on the phenomenological Minimal Supersymmetric Model (pMSSM) parametrization of supersymmetry and exemplify the constraining power of SMS results. We compare the official LHC Run-1 ATLAS results obtained for the same parametrization with the results obtained by SModelS, highlighting the gain in constraining power due to the use of both official and ‚homegrown‘ EM.

TUE23

17:00-17:15

Machine learning methods in the analysis of low-mass dielectrons in ALICE

Sebastian Lehner

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT

Results from non-perturbative QCD indicate that chiral symmetry may be restored in the hot and dense matter produced in relativistic heavy ion collisions. This restoration would affect the vector meson mass spectrum and could be examined with the ALICE detector at the LHC. One of the most promising probes to study these effects are dileptons ($\mu^+ \mu^-$ and $e^+ e^-$) from ρ meson decays since they reach the detector without significant final state interactions.

The main background in the analysis of dielectrons are combinatoric $e^+ e^-$ pairs ($S/B \sim 10^{-3}$). This background contribution can be suppressed by rejecting e^+ and e^- tracks that originate from photon conversion processes. Numerous observables allow to discriminate background from signal dielectrons which motivates a multivariate approach in the

classification of e^+e^- pairs. The employed machine learning methods and results obtained with Monte Carlo data will be presented as well as prospects for first low mass dielectron results on Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV.

LHS

CHRISTIAN-DOPPLER HÖRSAAL

ROMAN ULRICH SEXL PRIZE WINNER TALKS

CHRISTIAN-DOPPLER HÖRSAAL

TUE24

13:45-14:15

How Many Cultures of Knowledge are there?

Peter Schmid

University of Salzburg, Salzburg, AUT

Reflexions on the contribution of natural science to modern society: scientific knowledge as a component of interpreting the world and as a motor of technological progress.

The presence of science in the public discourse and in education: knowledge, competencies and understanding. Ethical limits on technical innovation.

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TUE25**14:15-14:45****Wissenschaft erzählen**Lothar Bodingbauer*Physikalische Soiree, Wien, AUT*

Der Roman Ulrich Sexl Preis geht 2016 an Lothar Bodingbauer für seine Arbeit an der „Physikalischen Soiree“. In dieser Radiosendung, die als Podcast weltweit verbreitet wird, spricht er mit Wissenschaftler/innen über ihre Forschungsarbeit. Als Radiojournalist arbeitet er auch für Österreich 1 und den Deutschlandfunk. In seiner Präsentation spricht er über die Verbindung von Wissenschaft mit Öffentlichkeit. Podcasts wie die Physikalische Soiree sind dabei eine ausgezeichnete Möglichkeit, für sendungsbewusste Wissenschaftler/innen, ein interessiertes Publikum zu finden. Allen Vermittlungsversuchen und -wünschen ist eines gemein: Es geht um Geschichten. Wie können Forschungsgeschichten zu den Menschen kommen. Worauf kommt es an, welche Zugänge sind denkbar, was ist schwierig und was funktioniert nicht gut.

**VWA Winner Talks
Christian-Doppler Hörsaal****14:45-15:15****Physics Olympiad
Christian-Doppler Hörsaal****15:45-16:00****International Young Physicists´ Tournament
Christian-Doppler Hörsaal****16:00-16:15**

YOUNG MINDS

CHRISTIAN-DOPPLER HÖRSAAL

TUE26

16:15-16:45

Let's get excited! Aufregung im sozialen Netz der Elektronen

Dominik Kreil

JKU Linz, Linz, AUT

In meiner Arbeit habe ich mir zur Aufgabe gemacht, die spannenden Wechselspiele zwischen Elektronen genau unter die Lupe zu nehmen. Wir kennen sie als Helfer, die durch die Kabel unserer Haushaltsgeräte sausen, und fürchten sie, wenn sie in Blitzen zur Erde fahren. Im Vergleich zu diesen Blitzen, sind die von mir studierten Ladungsträger in einer zweidimensionalen Welt gefangen. Ähnlich einem Wasserläufer auf der Oberfläche einer Pfütze, können sie sich nur in einer Ebene bewegen. Dies ist für ein Elektron durchaus nicht ungewöhnlich. Viele Computer-Bauteile sind heute so dünn, dass sich selbst die kleinsten Teilchen nur in zwei Richtungen frei bewegen können. Wichtig ist dabei auch, das Verhalten einer ganzen „Herde von Elektronen“ zu verstehen. Meist weichen sie einander aus und schirmen sich gegenseitig ab. Wie sich diese Elementarteilchen anziehen und abstoßen, hängt oft auch mit ihrer magnetischen Ausrichtung – dem sogenannten ‚Spin‘ – zusammen. Will man das Kollektiv aus der Ruhe bringen, stört man es mit elektrischen und magnetischen Feldern. Hierbei kann es dazu kommen, dass sich alle Elektronen gemeinsam bewegen. Um dieses Verhalten der Teilchen zu beschreiben, führte ich quantenmechanische Vielteilchenrechnungen durch. Meine Ergebnisse könnten zu leistungsfähigeren Bauteilen mit weniger Verlusten führen, insbesondere in der Spintronik: jene Technologie, welche Elektronik und die Nutzung des Spins kombiniert.

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TUE27

16:45-17:15**Schwarze Löcher - einfach oder kompliziert?**Jakob Salzer*Institute for Theoretical Physics, TU Vienna, Vienna, AUT*

Schwarze Löcher gehören zu den interessantesten und am häufigsten untersuchten Konsequenzen von Einsteins Allgemeiner Relativitätstheorie. Dennoch sind viele ihrer Eigenschaften noch immer nicht ausreichend verstanden. In diesem Vortrag möchte ich einige dieser Aspekte allgemeinverständlich erklären und erläutern, inwiefern das Verständnis schwarzer Löcher Hinweise auf eine Theorie der Quantengravitation liefern könnte.

TUE28

17:15-17:45**Spurenelementanalyse mit Totalreflexionsröntgenfluoreszenz**Aleksandra Winkler

Mirjam Rauwolf, Anna Turyanskaya, Johannes Sterba, Peter Wobrauschek, Christina Strelj

Atominstytut, TU Wien, Vienna, AUT

Die Totalreflexionsröntgenfluoreszenzanalyse (TXRF) ist ein Spezialverfahren der energiedispersiven Röntgenfluoreszenzanalyse (XRF). Sie ist eine zerstörungsfreie Multielementanalysemethode. Die Methode basiert auf der Anregung von Proben zu Emission von Fluoreszenzstrahlung im Röntgenbereich. Ist der Einfallswinkel kleiner als der kritische Winkel, so kommt es zur Totalreflexion auf der Probe und die Probe wird doppelt angeregt. Dadurch können auch sehr kleine Mengen von Proben gemessen werden. Dies macht die Methode sehr beliebt für Spurelementanalysen in z.B. Wasser- und anderen Umweltproben, sowie in Medizin und Biologie.

Gemessen wird bei der TXRF die von der Probe emittierte charakteristische Röntgenstrahlung. Da diese elementspezifisch ist, kann dadurch die Zusammensetzung der Probe bestimmt werden.

Um die Elemente in der Probe quantifizieren zu können, wird ein

interner Standard (ein vorher nicht in der Probe enthaltenes Element mit bekannter Konzentration) hinzugefügt.

Als Beispiel für die Messmethode werden Ergebnisse von Elementbestimmung in Kräuter- und Schwarztees gezeigt.

OGD
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JOSEF-STEFAN-HÖRSAAL
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TUE29

13:45-14:15

Single-Atom Catalysis - An Atomic-Scale View

Gareth Parkinson

TU Wien, Vienna, AUT

Single atom catalysis is a rapidly emerging but controversial area of catalysis research that aims to maximize the efficient usage of precious metals through the use of single atom active sites. Although catalytic activity has been demonstrated for several single atom catalyst systems, the inability to accurately characterize a catalyst based on single atom active sites ensures that that the field remains controversial, and little is really known about how a single atom adsorbed on a metal oxide support can catalyze a chemical reaction. In this lecture, I will describe how we are addressing the crucial issues of stability and reaction mechanism using a surface science approach. The work is based on the magnetite (001) surface, which exhibits an unusual reconstruction based on subsurface cation vacancies. A remarkable property of this reconstruction is that it stabilizes ordered arrays of metal adatoms (of almost any variety) with a nearest neighbor distance of 0.84 nm to temperatures as high as 700 K. Crucially, because the geometry of the adatoms is uniform and precisely known, reactivity experiments are performed on a well-defined model system, and theoretical calculations can be performed to shed light on the mechanisms underlying catalytic activity and deactivation. Several examples of our recent work will be used to illustrate the trends we have discovered to date,

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including how strong CO adsorption destabilizes Pd and Pt adatoms leading to mobility and rapid sintering, and how extraction of lattice oxygen from the metal-oxide is central to catalytic activity in the CO oxidation reaction.

TUE30

14:15-14:30**Single Rh adatoms at the Fe₃O₄ (001) surface and their interaction with gas molecules**

Roland Bliem (1)

Jessi E. S. van der Hoeven (2), Michael Schmid (1), Ulrike Diebold (1), Gareth S. Parkinson (1)

(1) Institut für Angewandte Physik, TU Wien, Vienna, AUT (2) Utrecht University, Utrecht, NED

Single-atom catalysis is a hot topic in catalysis research, aiming for high activity at optimum efficiency in the usage of precious metals. Understanding the reaction mechanisms in this emerging field requires atomic-scale information about the interaction of single metal adatoms with gas molecules. The Fe₃O₄ (001) surface is an ideal model system to study adatom-gas interactions as well as a promising support material for single-atom catalysis, because its ($\sqrt{2}\times\sqrt{2}$) R45° reconstruction [1] provides strong adsorption sites stabilizing single metal adatoms up to temperatures of 700K [2,3].

Here, we present a room-temperature study of Rh adatoms and their interaction with O₂, NO, CO, and H₂O using scanning tunnelling microscopy (STM) and density functional theory (DFT+U). Rh adatoms interact with each gas in a different way: O₂ adsorbs strongly, causing adatom mobility and sintering. NO adsorption also leads to mobility but hardly any cluster formation is observed. In contrast, the strong adsorption of CO does not induce mobility but poisons the adatoms' activity for O₂ adsorption. The complementary DFT calculations provide information on the binding strengths of O₂ and CO and metal-adsorbate bond lengths, enhancing the understanding of the processes observed in STM images.

[1] R. Bliem et al. Science 346, 1215-1218 (2014).

[2] Z. Novotny et al. Phys. Rev. Lett. 108, 216103 (2012).

[3] R. Bliem et al. ACS Nano 8, 7531-7537 (2014).

TUE31

14:30-14:45

Radio frequency scanning tunneling microscopy on molecular and atomic resonators

Stefan Müllegger

JKU Linz, Linz, AUT

To benefit from both, the high spatial resolution (~Å) of scanning tunneling microscopy (STM) and the exceptional energy resolution ($< \mu\text{eV}$) of magnetic resonance techniques, we have developed a spectroscopic radio frequency (rf) STM system. It enables the detection and excitation of mechanical [1,2] as well as spin [3,4] degrees of freedom in surface-adsorbed functional molecules with sub-nanometer spatial resolution. The contribution surveys recent showcases of rf-STM including the concerted mechanical oscillations of weakly coupled pi-radical molecules in the 100 MHz regime as well as the resonant excitation of single nuclear (I) and electronic (J) spin transitions up to 4 GHz in individual molecular quantum dots [3]. The latter have been found to occur unbound from electromagnetic dipole selection rules [4], i.e. exhibiting up to $\Delta I_z = \pm 3$ and $\Delta J_z = \pm 12$. The molecular quantum dots are formed by molecules of the single-molecule magnet bis-phthalocyanato terbium (III) and are studied either as individual single molecules on Au (111) or as molecular bilayer [5] at 5 K.

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

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

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

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

[5] G. Serrano, et al, J. Phys. Chem. C (in print). DOI: 10.1021/acs.jpcc.6b03676

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TUE32

14:45-15:00**On-surface synthesis and characterization of non-symmetrical single-molecule nodes**Christophe Nacci (1)

Andreas Viertel (2), Stefan Hecht (2), Leonhard Grill (1)

(1) Physical Chemistry Department, University of Graz, Graz, AUT (2) Department of Chemistry, Humboldt-Universität zu Berlin, Berlin, GER

On-surface reactions are a promising strategy for synthesizing complex architectures that are potentially relevant in the field of novel nanostructures and molecular electronics. Suitable design of molecular building blocks is required to construct specific molecular nanostructures of controlled geometry, symmetry and composition [1]. Low-temperature scanning tunneling microscopy is a powerful tool to image individual molecules at surface with high spatial resolution.

Molecular nodes linked to various entities play a key role in molecule-based electronic circuits, but represent a particular challenge because they require a well-defined arrangement of different building blocks. Here, we report the first construction of a chemically and geometrically well-defined covalent architecture made of one central node and three molecular wires arranged in a non-symmetrical fashion in order to ensure different conjugation pathways. Significant changes of the resulting synthesized molecular architectures are obtained by slightly modifying the molecular building blocks involved in the on-surface synthesis process on the Au (111) surface. The electrical characterization of individual non-symmetric molecular nodes by pulling them off a supporting surface with the tip of a scanning tunneling microscope will be discussed as well [2].

[1] L. Grill et al., Nature Nanotechnology 2, 687 (2007)

[2] L. Lafferentz et al., Science 323, 1193 (2009)

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TUE33

15:00-15:15

Reversible Control of Spin Transitions in a Magnetic Molecular Junction

Peter Jacobson (1)

Matthias Muenks (1), Oleg Brovko (2), Valeri Stepanyuk (2), Markus Ternes (1), Klaus Kern (1)

(1) Max Planck Institute for Solid State Research, Stuttgart, GER (2) Max Planck Institute of Microstructure Physics, Halle, GER

Model quantum systems such as adatoms and single molecular magnets on surfaces are prime targets for scanning tunneling microscopy and spectroscopy investigations. The magnetic behavior of these systems is usually defined by static parameters such as the local symmetry, the spin-orbit interaction, or the exchange coupling with the electron bath of the host. However, there is widespread interest in actively controlling molecular and adatom spin states for switching applications. Beyond imaging and spectroscopy, scanning probes are atomically precise manipulation tools. When manipulation and spectroscopy operate in tandem, it is possible to observe the formation of chemical bonds and continuously tune the exchange interaction between magnetic impurities. Despite some successes in actively controlling bonding and magnetic interactions between magnetic impurities, there are relatively few reports detailing how nanomagnets respond during manipulation events.

Here, we reversibly control the spin state of magnetic cobalt hydride complexes on a corrugated boron nitride surface with a scanning probe tip. Cobalt hydride complexes are made bistable with the impurity spin fluctuating between a correlated $S = \frac{1}{2}$ Kondo state, where host electrons screen the magnetic moment, and a $S = 1$ state with magnetocrystalline anisotropy. Combining conductance-distance and force-distance measurements together with density functional theory calculations, we unravel the microscopic potential energy landscapes present within the tunnel junction. Force measurements during switching shows that bonding between the cobalt hydride complex and the tip drives the spin transition. We demonstrate that by distributing the chemical functionality and reactivity between the tip and the undercoordinated adatom, the reactivity of the adatom can be harnessed to drive spin transitions.

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TUE34

15:45-16:15**Morphology and structure of ultra-thin silica films unveiled by spectro-microscopy**Thomas Schmidt*Fritz Haber Institute of the Max Planck Society, Berlin, GER*

For the understanding of the relationship between structure and reactivity of very complex catalytically active material systems like e.g. Zeolites, ultrathin SiO₂ and metal doped silicate films grown on a Ru (0001) support offer various possibilities as model systems. Preparation conditions and their influence on the Silica film properties were studied in situ with the aberration corrected spectro-microscope SMART at the synchrotron light source BESSY-II in Berlin, utilizing high-resolution XPEEM, μ XPS, valence band mapping, μ LEED and LEEM. The crystallographic and electronic structure of these SiO₂ films depend strongly on the deposited amount of Si and the oxidation conditions [1]. While the SiO₂ monolayer is strongly bound to the substrate, the SiO₂ bilayer film is of special interest, because it is only Van der Waals like bound and therefore lifts off the support. Depending on the preparation conditions, the bilayer is crystalline or vitreous [2] whereas the state can be transformed into each other. Under special conditions thicker SiO₂ films show an oxidation front, followed by oxygen intercalation. Moreover, with the possibility to desorb and intercalate gases under the SiO₂ bilayer, this film becomes an ideal model system to investigate chemical reactions in confined spaces [3].

[1] H.W. Klemm, G. Peschel, E. Madej, A. Fuhrich, M. Timm, D. Menzel, Th. Schmidt, H.-J. Freund, Surf. Sci. 643 (2016) 45 – 51

[2] L. Lichtenstein, C. Büchner, B. Yang, S. Shaikhutdinov, M. Heyde, M. Sierka, R. Włodarczyk, J. Sauer, H.-J. Freund, Angew. Chem. Int. Ed. 51 (2012) 404 - 407

[3] E. Emmez, B. Yang, S. Shaikhutdinov, H.-J. Freund, J. Phys. Chem. C 118 (2014) 29034 - 29042

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16:15-16:30

In-situ atomic-scale control of the growth of a polar perovskite oxide: SrTiO₃ (110) homoepitaxy by pulsed laser deposition

Michele Riva (1)

Stefan Gerhold (1), Bilge Yildiz (2), Michael Schmid (1), Ulrike Diebold (1)

(1) Institute of Applied Physics, TU Wien, Vienna, AUT (2) Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA

By combining pulsed laser deposition (PLD), high-pressure reflection high energy electron diffraction (RHEED), in-situ scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS), and low-energy electron diffraction (LEED), we investigate the homoepitaxial growth of SrTiO₃ on the (110) surface, from the first stages of sub-monolayer growth up to several nanometers-thick films.

The polar instability of the SrTiO₃ (110) surface is compensated by the formation of a variety of reconstructions, that can be finely tuned by adjusting the Sr and Ti content of the near-surface region [1]. The most stable surface structure, i.e., the SrTiO₃ (110) - (4 × 1) reconstruction, is part of a homologous series of (n × 1) (n = 4, 5, 6) reconstructions, and consists of a porous network of added TiO₄ tetrahedra [2, 3]. The Ti-richer (2 × 4) reconstruction, that exhibits a different symmetry and morphology, can co-exist with the (4 × 1) structure on the surface, upon appropriate sample preparation.

Islands grown by PLD on either (4 × 1) or (2 × 4) patches show a reconstruction, which is coherent with the one of the surrounding terrace, i.e., the substrate reconstruction segregates to the topmost layer. Analysis of STM images reveals that adspecies diffuse anisotropically on the SrTiO₃ (110) surface [4], with the preferential direction uniquely determined by the surface structure. The rotation in the high-mobility direction, combined with a reduced interlayer mass transport, result in the preferential accumulation of the deposited material at the 1D interface between (4 × 1) and (2 × 4) regions.

Deviations from the ideal Sr/Ti composition in the PLD flux are found to be detrimental for the morphological and structural quality of thick films: Sr-rich fluxes result in poor structural ordering at the surface of the grown films, while the preferential accumulation of the deposited material at (4 × 1) / (2 × 4) boundaries results in the development of

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deep pits with elevated rims for Ti-rich incoming fluxes. Reduction of these off-stoichiometries by optimization of the PLD parameters allows growing atomically-flat films with several nanometers thickness. The dependence of the surface structure on the near-surface composition, combined with the segregation of off-stoichiometries to the surface [5], allows the determination of the stoichiometry of the incoming flux with exquisite precision: by quantitative STM analysis of the change of the film structure upon growth, we obtain a resolution better than 0.5% in the Sr/Ti stoichiometric ratio. Support by the Austrian Science Fund FWF (SFB 'Functional Oxide Surfaces and Interfaces FOXSI' Project F45) and by the ERC Advanced Grant 'OxideSurfaces' (Project ERC-2011-ADG_20110209) is kindly acknowledged. SG acknowledges partial support by the FWF Doctoral College Solids4Fun, project number W1243.

Z. Wang, F. Yang, Z. Zhang, Y. Tang, J. Feng, K. Wu, Q. Guo, and J. Guo, Phys. Rev. B 83 155453 (2011). J. A. Enterkin, A. K. Subramanian, B. C. Russell, M. R. Castell, K. R. Poeppelmeier, and L. D. Marks, Nature Materials 9, 245 (2010). F. Li, Z. Wang, S. Meng, Y. Sun, J. Yang, Q. Guo, and J. Guo, Phys. Rev. Lett. 107, 036103 (2011). S. Gerhold, M. Riva, B. Yildiz, M. Schmid, and U. Diebold, submitted to Surf. Sci. J. Feng, F. Yang, Z. Wang, Y. Yang, L. Gu, J. Zhang, and J. Guo, AIP Advances 2, 041407 (2012).

TUE36

16:30-16:45**A novel SMSI mechanism driving the creation of ultra-thin zirconia (ZrO₂) layers**Peter Lackner

Joong-Il Jake Choi, Ulrike Diebold, Michael Schmid

TU Wien, Vienna, AUT

For oxide-supported metal catalysts, chemical reduction can lead to weaker H₂ and CO adsorption. This effect is known as strong metal-support interaction (SMSI) [1]. It was discovered that the effect was due to thin oxide films covering the metallic nano-particles serving as catalysts [2]. In most studies SMSI was only reported for reducible materials, where the thin films were formed by reduced material of the

supporting oxide. Later it was found that materials like ZrO₂, which is typically seen as non-reducible, can exhibit this SMSI effect [3]. Up to now the underlying mechanism was unclear.

We have prepared so-called inverse model-catalysts consisting of ZrO₂ islands on Rh (111) or Pt (111). Zr was deposited on the substrate using a UHV-compatible sputter source and annealed in oxygen to form ZrO₂ islands. In-between these islands the bare substrate remains. However, upon annealing under reducing conditions an ultrathin ZrO₂ (111) layer forms between the islands. This is the SMSI effect known from catalysis. We have investigated this system using X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). A new SMSI mechanism is proposed, which explains the formation of stoichiometric ultrathin films.

[1] Tauster, S. J. et al., Science 211, 1121-1125 (1981).

[2] Dulub, O. et al., Phys. Rev. Lett. 84, 3646 (2000).

[3] D. L. Hoang and H. Lieske, Catal. Lett. 27, 33 (1994).

TUE37

16:45-17:00

WO₃ Monolayer on Pd (100): formation of anti-phase domain boundary defects

Nassar Doudin (1)

D. Kuhness (1), M. Blattnik (1), Giovanni Barcaro (2), Alessandro Fortunelli (2), Falko P. Netzer (1), Svetlozar Surnev (1)

(1) Surface and Interface Physics, Institute of Physics, Karl-Franzens University, Graz, AUT (2) CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, Pisa, Italy

Tungsten trioxide (WO₃) is a key material in several applications including smart windows technology, photo-electrochemical water splitting, gas sensors and heterogeneous catalysis. In particular, tungsten oxides are important acid-base and redox catalysts, and they show excellent activity for many catalytic reactions, such as alcohol dehydrogenation, alkane hydrogenation and metathesis [1]. WO₃ has been produced in single crystal form or as supported thin films with the bulk crystal structure. Recently, the formation of an ordered two-dimensional (2D) tungsten oxide layer on Pt (111) has been reported, where W atoms

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show a mixture of 5+ and 6+ oxidation states [2]. Here we report on the preparation of a well-ordered 2D WO₃ layer on a Pd (100) surface and the characterization of its geometric, electronic and vibrational structure by a combination of STM, LEED, XPS, HREELS, supported by DFT calculations. The WO₃ monolayer on Pd (100) surface features a surface network consisting of small (~ 4 nm) square-shaped domains, separated by narrow (~ 0.3 nm) trenches. The latter are identified as anti-phase domain boundaries, as evidenced by atomically-resolved STM images and the characteristic spot splitting around the ($\pm 1/2$, $\pm 1/2$) LEED positions. The STM image shows that each domain exhibits a square surface structure with a lattice constant of 0.39 nm, which corresponds to a c (2x2) superstructure. Another important feature is the presence of few dark depressions inside the domains, which we attribute to missing terminal O atoms, in corroboration with HREELS results and high-resolution W 4f core-level spectra. The DFT derived structure model of the WO₃ monolayer consists of a layer of O atoms adsorbed in on-top Pd positions, followed by a c (2x2) layer of W atoms, which are connected at the top to terminal O atoms via strong W=O bonds, as suggested by the HREELS results. It can be viewed in a way as a 2D analogue of a cubic WO₃ (001) crystal, featuring a similar lattice constant (0.39 nm vs. 0.38 nm) and polyhedral linkage, but with a modified W-O coordination sphere due to the contact with the Pd (100) surface. The formation energy of the anti-phase domain boundaries has been studied in the DFT calculations as a function of the domain size. The most favourable domain size corresponds to 10 c (2x2) unit cells, in good agreement with the STM and LEED results. The DFT calculations reveal that the anti-phase boundaries geometry is, on the one hand, a means to minimize the surface strain, and on the other, to avoid the repulsive O-O interaction between neighbouring domains.

[1] D. Gazzoli et al, J. Phys. Chem. B 101 (1997) 11129 [2] Z. Li, et al, J. Phys. Chem. C 115 (2011) 5773 This work has been supported by the FWF Project P26633-N20.

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TUE39

13:45-14:00

Exponential communication complexity advantage from quantum superposition of the direction of communication

Philippe Allard Guérin

Adrien Feix, Mateus Araújo, Caslav Brukner

IQOQI/University of Vienna, Vienna, AUT

Quantum resources make it possible to solve certain communication and computation problems more efficiently than what is classically possible. In communication complexity problems, a number of parties wish to calculate a distributed function of their inputs while reducing the amount of communication between them. The minimal amount of communication is called the complexity of the problem. For some communication complexity tasks, the use of shared entanglement and quantum communication significantly reduces the complexity as compared to protocols exploiting shared classical randomness and classical communication.

In this work, we study the role in communication of a new resource: the quantum superposition of the ordering of parties. More precisely, we consider the process known as the quantum switch, in which a qubit coherently controls a superposition of „Alice before Bob“ and „Bob before Alice“. The quantum switch is known to provide advantages for certain computational tasks; it is also known to increase the success probability for some communication complexity task. However, up to now there was no known information processing task for which the quantum switch would provide an exponential advantage over causal protocols. We present a tripartite communication task for which such a superposition allows for an exponential saving in communication, compared to one-way quantum (or classical) communication. This is an SFB-FoQuS submission.

TUE40**14:00-14:15****Measuring time with physical clocks**Esteban Castro Ruiz

Flaminia Giacomini, Caslav Brukner

Faculty of Physics, University of Vienna, Vienna, AUT

In general relativity, the picture of spacetime assigns an ideal clock to each worldline. Being ideal, gravitational effects due to these clocks are ignored and the flow of time according to one clock is not affected by the presence of clocks along nearby worldlines. However, if time is defined operationally, as a pointer position of a physical clock that obeys the principles of general relativity and quantum mechanics, such a picture is at most a convenient fiction. Specifically, we show that the general relativistic mass-energy equivalence implies gravitational interaction between the clocks, while the quantum mechanical superposition of energy eigenstates leads to a non-fixed metric background. Based only on the assumption that both principles hold in this situation, we show that the clocks necessarily get entangled through time dilation effect, which eventually leads to a loss of coherence of a single clock. Hence, the time as measured by a single clock is not well-defined. However, the general relativistic notion of time is recovered in the classical limit of clocks. This is an SFB-FoQuS submission.

TUE41**14:15-14:30****Quantum mechanics with indefinite causal order**Flaminia Giacomini

Esteban Castro Ruiz, Caslav Brukner

Faculty of Physics, University of Vienna, Vienna, AUT

In all our well-established theories, it is assumed that events are embedded in a global causal structure such that, for every pair of events, the causal order between them is always fixed. However, the possible interplay between quantum mechanics and general relativity may require a revision of such a paradigm, for instance when the metric tensor,

and therefore the causal structure, is subject to quantum fluctuations. The process matrix framework is an operational approach to this question, and uses techniques typical of quantum information to address a problem which has been typically considered in quantum gravity. The framework retains the validity of quantum physics locally but doesn't assume the existence of a global causal order. For example, it allows to describe causal structures corresponding to a quantum superposition of 'A is before B' and 'B is before A'. The framework has been developed for both finite and infinite-dimensional Hilbert spaces. The long term goal is formulating quantum fields on indefinite causal structure, as required by the high-energy regimes at which the interplay between quantum mechanics and general relativity is expected. This is an SFB-FoQuS submission.

TUE42

14:30-14:45

Optimal Stochastic LOCC Transformations

David Sauerwein

Barbara Kraus

Institute for Theoretical Physics, University of Innsbruck, Innsbruck, AUT

Entanglement is the resource to overcome the natural restriction of spatially separated parties to Local Operations and Classical Communication (LOCC). It is at the heart of many quantum information tasks. We investigate here optimal stochastic LOCC (SLOCC) transformations of pure multipartite entangled quantum states. First, we show that deterministic transformations and the so-called One-Successful-Branch protocols (OSBPs) constitute the building blocks of all (to our knowledge) known optimal SLOCC protocols. We prove that the optimal probability to reach a state via an OSBP can be obtained by infinitely many different protocols, one being a protocol in which the initial state is probabilistically evolved into the final state via weak LOCC measurements. This transformation corresponds to a continuous path in the state space. These new insights allow us to find new optimal SLOCC protocols. Finally, we explore connections between the optimal conversion probability via SLOCC and physically meaningful distance measures among multipartite pure states.

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TUE43**14:45-15:00****Holography in Two- Dimensional Dilaton Gravity**Jakob Salzer*Institute for Theoretical Physics, TU Wien, Vienna, AUT*

The simplest toy models for classical and quantum gravity that can have black hole solutions are two-dimensional. Yet, two-dimensional Einstein gravity is not among them: in two dimensions the Einstein tensor vanishes identically and the Einstein-Hilbert action is a boundary term. Two-dimensional dilaton gravity provides a consistent theory of gravity in two dimensions. Among other applications, it presents an interesting testing ground for the conjectured duality between gravity theories in Anti-de Sitter spacetimes and gauge theories on the boundary. In this talk, I will introduce two-dimensional dilaton gravity and report on the study of holographic models in this set-up.

TUE44**15:00-15:15****Non-AdS Higher Spin Gravity**Stefan Prohazka*Institute for Theoretical Physics, TU Wien, Vienna, AUT*

The holographic principle, originally motivated by the extensive behavior of black hole entropy in one dimension lower than expected from a quantum field theory perspective, has found a concrete realization in the Anti-de Sitter/Conformal Field Theory (AdS/CFT) correspondence. One interesting testing ground for a more general correspondence is three-dimensional higher spin gravity. I will review higher spin gravity and show how non-AdS backgrounds can be constructed. Their boundary conditions and asymptotic symmetry algebras provide insights about possible dual theories which in turn could make non-AdS holography possible.

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TUE45

15:45-16:00

Peculiar Sonic Wave-Train Phase-Shift in Laminar Streaming Air

Karl Mocnik

Space Research Institute, Austrian Academy of Sciences, Graz, AUT

The phase-shift behaviour of a sonic wave-train along a given distance in laminar streaming air has been tested experimentally. Other than expected, the results seem to confirm the "Co-linear-Velocity-subtraction-Operation" (CVO), rather, than the well-known "Galilean-Velocity-subtraction-Operation" (GVO).

1. Karl Mocnik, „Experimental Test of the Frequency Change Characteristics of Laminar Streaming Air“, DAGA'90 (Deutsche Arbeits-Gemeinschaft für Aktustik, Wien 1990, Fortschritte der Aktustik), DAGA 16.1990, Wien, ISBN 3-923835-07-8.
2. Karl Mocnik, „Ein verkapptes Geometrieproblem und seine sieben Syllogismen“ Beiträge zum Mathematikunterricht, 45. Tagung für Didaktik für Mathematik, GDM (German Didactics of Mathematics), Freiburg, March 2011, S. 575-578. ISBN 978-3-942197-11-3.

TUE46

16:00-16:15

Space-, time- and frequency resolved recording and analysis of sound emissions and sound source localisation using a multichannel measuring system

Peter Wimberger (1)

Johann Emhofer (1), Christian Köfinger (1), Thomas Fleckl (2), Martin Gröschl (1), Christoph Reichl (1)

(1) AIT Austrian Institute of Technology, Vienna, AUT (2) TU Wien, Vienna, AUT

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To assess the acoustic behavior of heat pumps, a measuring system, consisting of a multichannel setup capable of simultaneous recording 64 microphone signals, an script-able adapted studio software and a thermal imaging camera, with two different microphone placement arrangement was set up and a software solution for evaluation was developed. One of those configurations is an acoustic camera, which allows visualization and evaluation of the sound sources' locations using beam forming methods. The second arrangement resembles a dome and enables the analysis of transient processes in the entire surrounding field of the heat pump. For long-term quantitative post-processing and visualization of the recording data a dedicated software with a graphical user interface was developed. The program allows space-, time- and frequency resolved analysis of the data to take appropriate measures to improve the acoustical properties. This can be done by implementation of insulation materials, optimization of internal processes such as reduction of the rotor speed or active noise controlling. On the basis of measurements of a heat pump used for educational purposes the possibilities of the two measurement configurations are demonstrated. The analysis of the data generated by the acoustic camera allows visualization of the sound sources directly on a computational model of the heat pump. The measurements made with the dome show a directional characteristic of sound emission based on the asymmetrical arrangement of the acoustical significant components compressor and fans. SilentAirHP is supported in the framework of the „Energy research program of the Climate and Energy Fund“ first call (5148527) initiated by the Austrian Ministry for Transport, Innovation and Technology (BMVIT)

TUE47

16:15-16:30**SilentAirHP - Advanced Methods for Analysis and Development of Noise Reduction Measures for Air-to-Water Heat Pump Systems**Christoph Reichl

Johann Emhofer, Christian Köfinger, Thomas Fleckl

AIT Austrian Institute of Technology, Vienna, AUT

Due to their multiple advantages such as low investment costs and low

space requirements air-water-heat pumps became very popular within recent years representing now the best-selling pump system for heating and cooling residential buildings on a European-scale. Besides the disruptive noises of the compressor, unpleasant sound is mainly generated by the fan and the evaporator as a result of the required high air flow rate of air-water-heat pumps. Especially in the transitional period when icing of the evaporator occurs, an additional noise emission takes place leading often to neighbourly conflicts. This might become a competitive disadvantage of this technology hampering its broad dissemination particularly in densely populated areas. The noise reduction actions discussed in literature and acoustic guidelines of heat pump manufacturer associations, etc. comprise constructive, component-specific, control-wise and active measures evaluating the measures' effect on the noise level on a qualitative scale only. As the concurrent effects of these sound reducing measure (s) on performance, COP, noise emission and psychoacoustic perception are currently not assessed on a quantitative level, heat pump manufacturers, installers and planers are not aware which of the conventional actions are the most promising for their heat pump system as a whole. The project SilentAirHP therefore aims at developing respectively adapting advanced numerical and experimental methods for the assessment of noise-reducing measures for air-water-heat pumps. Sound measurement methods able to localize sound sources frequency-resolved, overall-system simulations considering sound emissions also during the icing of the outdoor unit, and control-wise measures are developed and experimentally tested on an industry-oriented modular air-water heat pump system. Besides the quantification of selected passive measures, the effect of anti-ice-coatings developed by the WYSS Institut (Harvard University) during icing and defogging on the noise level and noise cancelling as active measure will be tested and assessed. In cooperation with the Acoustic Research Institute of the Austrian Academy of Sciences, selected noise reduction measures are assessed psychoacoustically. The results will comprise a set of quantitatively analysed actions for known and innovative noise reduction measures evaluated on an energetic and noise level. Furthermore a comprehensive system description of an air-water heat pump system considering the icing behaviour and the noise emission simultaneously for the first time will be generated in the course of the program. The presentation sets the scope of the October 2015 started three years project. Futhermore, current actions taken to initiate a

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worldwide research collaboration in the framework of the IEA heat pump implementing agreement are outlined. SilentAirHP is supported in the framework of the „Energy research programm of the Climate and Energy Fund“ first call (5148527) initiated by the Austrian Ministry for Transport, Innovation and Technology (BMVIT)

TUE48**16:30-16:45****Active Noise Cancelling fro Heat Pump Applications**Norbert Schmiedbauer (1)

Johann Emhofer (1), Christian Köfinger (1), Peter Wimberger (1), Thomas Fleckl (1), Martin Gröschl (2), Christoph Reichl (1)

(1) AIT Austrian Institute of Technology, Vienna, AUT (2) TU Wien, Vienna, AUT

Active Noise Cancelling (ANC) is used in the research project „SilentAirHP“ as an attractive and promising method to reduce the acoustic emissions of air-to-water heat-pumps. This method is primarily used in ANC-headsets, several applications, however, are also available in the automotive and aeronautic industry. The ANC principle is known since around 1930, but gets more and more applicable due to the advent of fast and light signal processing units. An unwanted sound source is recorded with a microphone. The microphone signal is analyzed in real time using a processor and a phase inverted (anti-noise) signal is generated and emitted using a well-placed loud speaker. The original signal mixes with the anti-noise signal ideally producing a destructive interference. In the real world, extinctions will never be perfect and thus only a partial reduction can be achieved. The degree of emission reduction furthermore depends on the position of the observer. The long term goal is to assess the applicability of ANC in the field of air-to-water heat pumps. Installation, adaption, tests and optimum coupling to the structure of the unit plays a vital part. To reach this target, the control of the unit and the achievable reduction of the acoustic emissions is demonstrated using a rectangular channel consisting of a fan, a microphone and a loudspeaker. A multichannel acoustic measurement system (acoustic dome) is used to capture the transient, space-, and frequency-dependent acoustic waves. Analysis of the data allows for quantification of the achievable reduction potential in the different acoustic

bands. Furthermore, an acoustic camera is utilized to visualize the effect of the ANC module on the sound source distribution on the unit. The temperature dependence of the ANC setup as well as the microphone measurement equipment is tested using the climatic chambers at AIT (Austrian Institute of Technology). This is important, as heat pumps have to be acoustically characterized in several climatic conditions. Transient features in acoustic emissions are commonly observed during icing of the evaporator which is typically observed in high humidity near zero degree scenarios. SilentAirHP is supported in the framework of the „Energy research program of the Climate and Energy Fund“ first call (5148527) initiated by the Austrian Ministry for Transport, Innovation and Technology (BMVIT)

TUE49

16:45-17:00

In-situ measurement and simulation of acoustic noise barrier parameters

Harald Ziegelwanger

Marco Conter, Paul Reiter, Reinhard Wehr

AIT Austrian Institute of Technology, Vienna, AUT

Noise barriers are the primary mean in noise abatement for traffic-related noise in the proximity of roads and railways. The acoustic properties of noise barriers are characterized by intrinsic parameters, i.e., the sound reflection index, the sound insulation index, and the sound diffraction index, and by extrinsic parameters, i.e., the insertion loss. The intrinsic parameters can be measured in-situ (according to EN 1793-4, EN 1793-5, and EN 1793-6 for road noise and according to EN 16272-4, EN 16272-5, and EN 16272-6 for railway noise) or calculated from results of acoustic simulations. While the reflection index and the insulation index require the simulation of the interior structure of a noise barrier, e.g., by the finite element method (FEM), the diffraction index and the insertion loss can be calculated from simulation results of the boundary element method (BEM).

The standards EN 1793 and EN 16272 define the frequency range, i.e., frequencies up to the 5 kHz third-octave band, for the measurement and, thus, for the simulations. However, the computational cost of

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the acoustic simulation tools increase with the frequency and the size of the simulated noise barrier. Thus, noise barrier models have to be simplified in order to calculate the sound field for the standardized frequency range. A common approach is to simplify a noise barrier model to its cross section and to use the two-dimensional BEM (2D-BEM) for the simulation. However, the 2D-BEM limits the geometry to noise barriers with a one-dimensional constant profile. An interesting compromise solution between 2D-BEM and 3D-BEM is the quasi-periodic BEM. The QP-BEM allows the simulation of periodically repetitive complex three-dimensional structures while keeping the computational cost at a reasonable level. Also the complexity of finite element models can be reduced to periodic unit cells by applying periodic boundary conditions. In this presentation, we first review the in-situ measurement techniques for the different intrinsic parameters, the periodic FEM formulation and the quasi-periodic BEM. Then, we show simulation results for noise barrier components and compare the results to in-situ measurements. For noise barrier top elements, we also show their effect on the insertion loss.

TUE50

17:00-17:15**Simulation of Railway Vibrations**Holger Waubke*Acoustics Reserch Institute, Austrian Academy of Sciences, Vienna, AUT*

In tunnels, vibrations are the only annoying emissions from railway traffic. A tool is presented that allows to simulate the waves in a stratified anisotropic linear elastic medium. The boundary element method is used for the soil. The tunnel shell is simulated using analytical solutions for a plane shell element in 2.5D. The tunnel shell is coupled with the boundary element method assuming constant stresses at the boundary that are coupled with the pressure loads of the shell elements. The displacements are coupled at the nodes. One disadvantage of the method are the singular integrals in the boundary element method at the positions of the test functions, because the solution is only known numerically. A change of the order of element integration assuming constant or linear shape functions and the inverse Fourier

integral transformation allows to solve the element integrals analytically. The result is an attenuation of the spectra that can now be transformed numerically.

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TUE51

13:45-14:00

Wave-Particle Duality and Optical Correlations

Mayukh Lahiri (1)

Armin Hochrainer (1), Gabriela Lemos (1), Radek Lapkiewicz (2), Anton Zeilinger (1)

(1) IQOQI/University of Vienna, Vienna, AUT (2) University of Warsaw, Warsaw, POL

Wave-particle duality, which is a key feature of quantum mechanics, is directly connected to the ability of a quantum entity to interfere [1]. If a quantum entity is sent through a two-path interferometer and one can identify the path it traverses, no interference occurs. The availability and unavailability of the which-path information are usually referred to as the particle and the wave behaviors of the quantum entity, respectively. Several theoretical studies have been conducted on the relationship between the which-path information and visibility of fringes in interference experiments [2-4]. This relationship has been convincingly demonstrated in 1991 [5] and has recently been applied to develop a quantum imaging technique [6].

According to the coherence theory of light, the visibility of an interference pattern is governed by the correlation between the interfering optical fields [7]. Furthermore, optical field correlations have also been shown to govern the polarization properties of light [7]. In this talk, we present the results of an experiment which demonstrates that the degree of polarization of a light beam emerging from an output of an interferometer depends on the which-path information. A remarkable feature of the experiment is that, without interacting with the beam, we

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are able to change the beam from being fully polarized to being fully unpolarized. We for the first time provide quantitative evidence that a connection between partial polarization and wave-particle duality exists. Our results thus give new insights into the relationship between wave-particle duality and optical field correlations.

[1] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics*, Vol. III, (Addison-Wesley Publishing Company, New York, USA 1966).

[2] D. M. Greenberger and A. Yasin, "Simultaneous wave and particle knowledge in a neutron interferometer," *Phys. Lett. A* 128, 391-394 (1988).

[3] L. Mandel, "Coherence and indistinguishability," *Opt. Lett.* 16, 1882-1883 (1991).

[4] B-G. Englert, "Fringe visibility and which-way information: an inequality," *Phys. Rev. Lett.* 77, 2154 (1996).

[5] X. Y. Zou, L. J. Wang, and L. Mandel, "Induced coherence and indistinguishability in optical interference," *Phys. Rev. Lett.* 67, 318-321 (1991).

[6] G. B. Lemos et al, "Quantum imaging with undetected photons," *Nat.* 512, 409-412 (2014).

[7] L. Mandel, and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, Cambridge, 1995).

TUE52

14:00-14:15

Ultracold atoms on superconducting atomchips

Stefan Minniberger

Atominstytut, TU Wien, Vienna, AUT

Superconducting atomchips are a promising tool in atom optics and are studied in various groups all over the world. They provide some advantages over their normal conducting counterparts, such as reduced Johnson-Nyquist noise from the wires and the possibility to create a self-sufficient traps without any external connections, therefore being free from technical noise. The cryogenic environment also comes with technical advantages like long lifetime and rapid reconfigurability due to effective cryo-pumping, allowing to replace the atomchip in a matter

of days rather than months. Superconducting atomchips can be used to realize a hybrid quantum system with the long-lived hyperfine states of ultracold atoms and the excitations in a superconducting microwave cavity. The microwave cavity can either be formed by a lambda-half resonator or a lumped element resonator, placed on the same chip as the trapping wires. Vortices penetrating type-II superconductors can be used to create almost arbitrary arrays of magnetic microtraps. These trap arrays can be scaled down to a range where we are able to compete with optical lattices, with the ultimate goal being a trap array formed by the vortex lattice of a fully magnetized superconductor. A detailed understanding of the particularities of superconducting atomchips is necessary to make full use of their potential. The current distribution in a type-II superconductor strongly depends on the history of applied fields and currents and can therefore be tailored, allowing to change the effective wire width and to reach very small distances between the wire and the atom cloud, where surface interactions can be studied.

TUE53

14:15-14:30

Towards arbitrary optical dipole potentials for one-dimensional quasi-condensates

Mohammadamin Tajik

Bernhard Rauer, Thomas Schweigler, Federica Cataldini, Kaspar Sakmann, Jörg Schmiedmayer

Atominstitut, TU Wien, Vienna, AUT

We are using a Digital Micromirror Device to realize arbitrary static and dynamic optical dipole potentials for one-dimensional (1d) quasi-condensates of 87Rb created on an atomchip. This approach of a hybrid optical and magnetic trap combines the high flexibility of optical dipole traps with the advantages of magnetic trapping, such as effective evaporative cooling and the application of rf dressed state potentials. This system allows us to investigate the dynamics of 1d quantum systems more deeply and to address exciting questions in quantum thermodynamics and quantum information.

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TUE54

14:30-14:45

Three photon energy-time entanglement from cascaded down conversion

Thomas Kauten (1)

Sascha Agne (2), Jeongwan Jin (2), Deny Hamel (3), Evan Meyer-Scott (2), Jeff Salvail (2), Kevin Resch (2), Gregor Weihs (1), Thomas Jennewein (2)

(1) Institut für Experimentalphysik, University of Innsbruck, Innsbruck, AUT (2) Institute for Quantum Computing, University of Waterloo, Waterloo, CAN (3) Departement de Physique et d'Astronomie, Université de Moncton, Moncton, CAN

Entangled photons are a key requirement for realizing worldwide quantum communication [1]. Those photon pairs are used for various applications such as quantum cryptography and optical quantum computation. The photons can be entangled in various degrees of freedom, usually the photons are polarization entangled, since it is relatively easy to realize. Unfortunately, these photons have limited transmission length through fibers due to polarization mode dispersion. Therefore the photons have to be entangled in a different, more robust degree of freedom; in this case we use energy-time entanglement [2]. For some application it is also required to have more than two photons entangled; we are therefore demonstrating the creation of energy-time entangled photon triplets via cascaded parametric down conversion. Our source creates approximately 2000 entangled photon triplets per hour [3]. We analyze the photon triplets with three imbalanced Mach-Zehnder interferometers where we were able to observe three-photon interference with a visibility of $(63.6 \pm 7.5) \%$, while having negligible two-photon and single-photon modulation. In order to prove entanglement we try to violate Mermin's inequality [5], the generalized Bell inequality for more than two particles.

[1] Kimble, Nature 453, 1023-1030 (2008)

[2] Franson, Phys. Rev. Lett. 62, 2205 (1989)

[3] Shalm et al., Nature Physics: 9, 19 (2013)

[4] Hübel et al., Nature 466, 601-603 (2010)

[5] Mermin, Phys. Rev. Lett. 65, 1838 (1990)

TUE55

14:45-15:00

Single-atom-controlled, fiber-integrated optical circulator

Michael Scheucher

VCQ, Atominstitut, TU Wien, Vienna, AUT

Nanophotonic components confine light at the wavelength scale and enable the control of the flow of light in an integrated optical environment. The strong confinement of light leads to an inherent link between its local polarization and propagation direction - the light obtains a chiral character - and thereby fundamentally alters the physics of light-matter interaction [1].

We employ this effect in order to investigate the realization of novel nonreciprocal optical devices that operate at the single-photon level. For this purpose, we use a single spin-polarized 85Rb atom that is strongly coupled to a novel type of whispering-gallery-mode microresonator - a so-called bottle microresonator [2]. These resonators offer the advantage of being fully tunable and provide very long photon lifetimes in conjunction with near lossless coupling to the nanofibers. This renders them ideal for the investigation of nonreciprocal light propagation based on chiral light-matter interaction.

As a first application, based on chiral interaction of light and matter, we realized an optical diode whose directional behavior is controlled by the internal state of a single atom. We observe a strong imbalance between the transmissions through the fiber in forward and reverse direction of 13 dB [3]. By interfacing the bottle microresonator with two nanofibers we extended this system to a 4-port device, where photons are nonreciprocally directed from one fiber port to the next, forming an optical circulator. For an optimized setting, we managed to show a mean isolation of 7 dB for the four relevant direction. Since our circulator is, in contrast to the diode, based on a non-dissipative process we still maintain a high photon survival probability of 70%. Furthermore, the sense of circulation can be inverted by changing the state of the atom, realizing a programmable circulator. These properties enable such a circulator to be used in quantum information protocols. In my talk I will explain the underlying principles of such an optical circulator and present a full characterization of our nonreciprocal device.

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- [1] C. Junge et al., Phys. Rev. Lett. 110, 213604 (2013).
- [2] M. Pöllinger et al., Phys. Rev. Lett. 103, 053901 (2009).
- [3] C. Sayrin et al., Phys. Rev. X 5, 041036 (2015).

TUE56

15:00-15:15

Scalable control and sensing with quantum defects in semiconductors

Michael Trupke

VCQ, Atominstitut, TU Wien, Vienna, AUT

Spin systems in semiconductors such as silicon, diamond and silicon carbide are promising candidates for the physical implementation of quantum bits. In particular, the nitrogen-vacancy defect in diamond has garnered significant attention in recent years due to long spin coherence times, even at room temperature [1]. Under cryogenic conditions, the defect presents optical transitions similar to those of simple molecules, enabling its use as a practical interface between stationary spins and flying photonic qubits.

Two-frequency pulses are powerful tools for the manipulation of multi-level quantum systems [2]. I will describe their application to magnetometry using nitrogen-vacancy centres in diamond [3]. We have demonstrated both multi-axial and numerically optimised pulsed sequences for the 3-level ground state, enabling the most sensitive measurement method for quasi-static and oscillating magnetic fields to date using a single spin in diamond. We have found that the single-spin sensitivity to magnetic fields can be improved in isotopically purified diamond by making use of states with extended coherence times in the spin-1 manifold. Furthermore the long-term stability of magnetic field measurements is significantly enhanced, leading to a reduction of the minimum detectable field variations. We demonstrate sensitivities of 8 nT/ $\sqrt{\text{Hz}}$ and 2.2 nT/ $\sqrt{\text{Hz}}$ for quasi-static and oscillating fields, with a long-term noise floor below 800 pT and 50 pT, respectively. The manipulation methods used herein furthermore enable efficient control over the NV qutrit manifold.

Finally, I will describe the use of two-frequency manipulation for the control of spin qubits in large-scale quantum information registers [4]. The manipulation protocol leads to a quadratic reduction in the

required control resources, and is applicable to a broad variety of spin qubits in semiconductors. First experimental results using microfabricated control structures on a diamond chip will be presented.

[1] M. W. Doherty et al., The nitrogen-vacancy colour centre in diamond. *Phys. Reports* 528 1, 1-45 (2013).

[2] K. Bergmann, H. Theuer, and B. W. Shore. Coherent population transfer among quantum states of atoms and molecules. *Rev. Mod. Phys.* 70 3, 1003 (1998).

[3] A. Angerer, T. Nöbauer, G. Wachter, M. Markham, A. Stacey, J. Mayer, J. Schmiedmayer and M. Trupke. Subnanotesla quantum-interference magnetometry with a single spin in diamond. arXiv:1509.01637 (2015).

[4] K. Nemoto, M. Trupke, S. J. Devitt, A. M. Stephens, K. Buczak, T. Nöbauer, M. S. Everitt, J. Schmiedmayer, W. J. Munro. Photonic architecture for scalable quantum information processing in diamond. *Phys. Rev. X* 4 3, 031022 (2014).

TUE57

15:45-16:00

Relaxation of a Bose-Einstein condensate from a coherent superposition of vibrational levels

Marie Bonneau

Sandrine van Frank, Mira Maiwöger, Raisa Trubko, Marine Pigneur, Rugway Wu, Thorsten Schumm, Jörg Schmiedmayer

TU Wien, Vienna, AUT

Understanding the non-equilibrium dynamics of quantum many-body systems is an open problem, common to systems with very different length, time and energy scales, ranging from cosmology to ultracold gases. We consider here the relaxation dynamics of a 1D Bose gas prepared in a coherent superposition of the first two transverse vibrational levels of the trapping potential.

The system is initialized through optimal control of the displacement of the anharmonic transverse potential [1]. This method permits fast preparation of excited motional states with 99% fidelity and is robust towards atom number fluctuations [2]. Experimental characterization of the non-equilibrium evolution was performed. The system evolves

towards a steady state, with a characteristic timescale strongly depending on the atom number of the Bose gas. We investigated the contribution to the relaxation of several effects: Local fluctuations of the vibrational levels' relative population arise during the system initialization, leading to prethermalization through propagation of relative density and relative phase excitations, in a similar fashion as observed for symmetrically split 1D gases [3].

Another source of longitudinal dephasing is the finite longitudinal coherence of the 1D gas, which results in fluctuations of the relative phase due to the asymmetry of the levels' sound velocities. Additionally, emission of atom pairs from the excited vibrational level [4] triggers many-body dephasing.

[1] van Frank et al., Nat. Commun. 5, 4009 (2014).

[2] van Frank et al., arXiv:1511.02247 (2015).

[3] Gring et al, Science 337, 1318 (2012).

[4] Bücker et al., Nat. Phys. 7, 608–611 (2011).

TUE58

16:00-16:15

Recurrence of an isolated quantum many-body system

Bernhard Rauer (1)

Sebastian Erne (1), Thomas Schweigler (1), Federica Cataldini (1), Jörg Schmiedmayer (1), Thomas Gasenzer (2)

(1) Atominstytut, TU Vienna, Vienna, AUT (2) Institut für Theoretische Physik, Universität Heidelberg, Heidelberg, GER

Isolated quantum many-body systems undergoing unitary time evolution are expected to rephase back to their initial state after a certain time. Yet for typical systems with incommensurate eigenenergies and many degrees of freedom this time is tremendously long prohibiting the observation of such recurrences. We show however, that in a system that can effectively be described by only a few commensurate modes a revival of the initial state is not only a gedankenexperiment but lies within experimental reach.

Our model system is a pair of tunnel-coupled one-dimensional quasi-condensates which we take out of equilibrium by a fast ramp-down

of the tunnel-coupling. In the subsequent evolution the relative phase field of the two condensates is monitored, providing a local probe for the system. This allows us to directly observe how the initial phase coherence between the two many-body systems is first lost and later reemerges to a partial recurrence of the initial state.

TUE59

16:15-16:30

Optimal state estimation for cavity optomechanical systems

Witlief Wieczorek (1)

Sebastian G. Hofer (1), Jason Hoelscher-Obermaier (1), Ralf Riedinger (1), Klemens Hammerer (2), Markus Aspelmeyer (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Leibniz University Hannover, Hannover, GER

How does one optimally estimate the state of an optomechanical system? This can be done with Kalman filtering, which is a method known from signal processing with the goal to estimate the state of a linear Gaussian system. Kalman filtering is widely applied for classical purposes such as navigation and tracking. We demonstrate the application of Kalman filtering in a new domain: for estimating the optomechanical state in a cavity optomechanical system. In our case, a micromechanical cantilever is coupled to a high-Finesse optical cavity, both in the weak and strong coupling regime. The Kalman filter we utilize hinges upon a realistic state-space model, which takes into account nontrivial experimental noise sources. Most importantly, we check the validity of our approach by characterizing the innovation sequence, which captures the difference of actual measurements and measurement predictions. The application of the Kalman filter in the domain of optomechanics is manifold: feedback control, conditional cooling, mechanical sensing or estimation of the optomechanical quantum state. The use of the Kalman filter may thus provide a significant advantage for quantum control experiments of massive mechanical systems.

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TUE60**16:30-16:45****Model calculations for coherent optical transfer in alkali-strontium molecules**Johann V. Pototschnig

Ralf Meyer, Andreas W. Hauser, Wolfgang E. Ernst

Institut für Experimentalphysik, TU Graz, Graz, AUT

Recently, ultracold heteronuclear molecules in low vibrational levels of the electronic ground state have been produced by Feshbach resonance techniques and a subsequent coherent optical transfer.[1] These molecules have a permanent electric dipole moment, but no magnetic dipole moment. In contrast, combinations of alkali and alkaline earth atoms show both types of dipole moments, offering the prospect of increased control in experimental setups. In this study, we focus on the group of AK-Sr (AK=Li, Na, K, Sr) molecules for a preliminary investigation. We start by performing ab initio computations for these molecules with three different methods (MRCI, CASPT2, EOM-CCSD) and compare the resulting potential energy curves for the lowest seven electronic states. Subsequently, we determine the Franck-Condon factors and transition probabilities for different vibronic states, and use these results to discuss possible optical transfer schemes that might become important for molecular formation at ultracold temperatures.

[1] K. K. Ni et al., Science 322, 231 (2008)

TUE61**16:45-17:00****Measuring Spin Relaxation with Novel 3D Lumped Element Cavities**Thomas Astner*Atominstytut, TU Wien, Vienna, AUT*

Transmission line (stripline) cavities and three dimensional cavities are the most prominent design for cavityQED experiments in the microwave regime. However, when coupling large solid state spin ensembles to such cavities, they suffer from the large field gradient in the sample,

resulting in an inhomogeneous coupling strength for each spin in the ensemble with the cavity mode. These inhomogeneous single spin Rabi frequencies make it impossible to coherently manipulate and control the whole ensemble. Here we show the design of a 3D lumped element cavity for cavityQED experiments which overcomes this limitation and demonstrate a new technique for measuring the longitudinal relaxation time of a large nitrogen vacancy spin ensemble.

TUE62

17:00-17:15

Laser cooled anions as a sympathetic coolant

Julian Fesel

CERN, Genève, SUI

At CERN there are currently several experiments under way that aim at examining the CPT theorem and the weak equivalence principle using antimatter, among them the AEGIS experiment. For the latter, antihydrogen is formed from antiprotons inside a Penning trap via positron attachment, which is then used for precision measurements. The experiments are currently limited by the temperature of the antiprotons, which influences the antihydrogen temperature and consequently the sensitivity of the experiments. In order to cool the antiprotons, we are working on a scheme using laser-cooled anionic molecules for sympathetic cooling of the antiprotons. I will present our design for a C₂- source, that produces pulses of cold molecules in the ground state and will discuss further steps and possible schemes for laser cooling of this anion species inside a Penning trap.

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FRITZ KOHLRAUSCH PRIZE WINNER TALK

LISE-MEITNER-HÖRSAAL

TUESDAY

WED00

11:00-11:30

Taming single atoms - and teaching them math

Thomas Monz (1)

D. Nigg (1), E. A. Martinez (1), R. Stricker (1), A. Erhard (1), P. Schindler (1),
R. Blatt (1,2)

*(1) Institute of Experimental Physics, University of Innsbruck, Innsbruck, AUT (2) Institute for
Quantum Optics and Quantum Information, Austrian Academy of Sciences, Innsbruck, AUT*

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Only about a century ago, physicists were trying to understand what matter consists of, and which rules govern its behavior. Today, students routinely work with atoms and ions, a few at a time as well as entire ensembles, without a second thought. Control of these systems has reached a point where both internal and external properties of an atom are manipulated with the push of a button. This presentation focuses on trapped ions, and explains how these are stored, manipulated, and turned into the building blocks of a quantum computer located in Innsbruck. Subsequently the first realization of mathematical operations in a quantum computer is explained and the implementation of Shor's algorithm illuminated. The presentation concludes with an outlook towards our first steps for fault-tolerant quantum computing and how such a system is currently being connected to a quantum network.

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ÖPG Plenary Assembly Lise-Meitner-Hörsaal

11:30-12:30

COND/NESY

LUDWIG-BOLTZMANN-HÖRSAAL

WED01

13:45-14:15

Decomposition of pseudomorphic Ge_{1-x}Sn_x alloys grown on Ge (001)

Heiko Groiss (1)

Martin Glaser (2), Magdalena Schatzl (2), Moritz Brehm (2), Friedrich Schäffler (2)

(1) CDL-MS-MACH, Center for Surface and Nanoanalytics, Linz, AUT (2) Institute of Semiconductor and Solid State Physics, Linz, AUT

The integration of light sources with Si microelectronics is an essential step towards integrated optical communication and on-chip optical interconnects. Recently, a breakthrough was achieved with the demonstration of lasing in strain-relaxed GeSn epilayers [1, 2]. Despite this major achievement, the thermal stability of Ge_{1-x}Sn_x films with Sn contents far above the solid solubility limit of ≈0.5% remains a concern regarding the high processing temperatures of up to 1000°C routinely employed during the fabrication of Si integrated circuits.

We investigated Ge_{1-x}Sn_x epilayers grown by MBE at low temperatures (down to 120° C) and at high growth rates of 1 Å/s⁻¹ to implement Sn contents of more than 14 percent in fully coherent, single crystalline epilayers. Pseudomorphic growth was demonstrated on Ge (001), SiGe/Si and Si/SOI substrates. For the latter also the growth of relaxed GeSn layers could be shown. The structural properties of the samples were characterized by X-ray diffraction. TEM experiments were used

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to investigate the onset of phase separation in these metastable films with high Sn content.

To assess the thermal stability and the precipitation kinetics of the epilayers under well-controlled experimental conditions we use series of un-capped $\text{Ge}_{1-x}\text{Sn}_x$ films on commercial Ge (001) substrates. These films were either grown at different growth temperatures up to 400°C , or grown at low temperature and subsequently annealed in-situ in the environment of the MBE chamber, again at temperatures up to 400°C . Additionally, a similar series was grown, but annealing was performed ex-situ in the vacuum environment of a scanning electron microscope (SEM) with a heatable sample holder. In all three cases we found strong decomposition effects above the β -Sn melting point of $T_m = 231.1^\circ\text{C}$. The most spectacular effect is the formation of β -tin droplets, which are moving over the uncapped surface. Thereby, they collect by a ripening mechanism Sn from the metastable layer, leaving behind a rough surface, which shows self-avoiding trails with a distinct pattern of droplet movement along crystallographically preferred directions.

We compiled video sequences of the process from the in-situ SEM experiments. In addition, the developing structure was analyzed by AFM and extended TEM measurements. After cool-down, Sn precipitates of different orientations with respect to the substrate were found. Most of the layer's Sn content is accumulated in these Sn precipitates, leading to an essentially strain-relaxed Ge layer in the trail of each moving droplet. In front of the moving droplet, the film remains fully strained with its original Sn concentrations. This concentration- and strain-gradient provides the driving force for droplet movement and explains the self-avoiding trails.

[1] K. P. Homewood, M. A. Lourenço, „Optoelectronics: The rise of the GeSn laser“, *Nature Photonics* 9, 78–79, (2015), doi:10.1038/nphoton.2015.1

[2] S. Wirths, R. Geiger, N. von den Driesch, G. Mussler, T. Stoica, S. Mantl, Z. Ikonc, M. Luysberg, S. Chiussi, J. M. Hartmann, H. Sigg, J. Faist, D. Buca, D. Grützmacher, „Lasing in direct-bandgap GeSn alloy grown on Si“, *Nature Photonics* 9, 88–92, (2015) doi:10.1038/nphoton.2014.321

WED02

14:15-14:45

Observation of multi-wavelength neutron Pendellösung interference in holographic nanostructures

Jürgen Klepp (1)

Martin Fally (1), Peter Geltenbort (2), Christian Pruner (3), Yasuo Tomita (4)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Institut Laue Langevin, Grenoble, FRA (3) University of Salzburg, Salzburg, AUT (4) University of Electrocommunications, Tokyo, JPN

Previous experiments with nanoparticle-polymer composite grating-structures fabricated by optical holography have demonstrated how they can be used as multi-port beam-splitters or mirrors for cold and very-cold neutrons. In a recent experiment, we have observed the Pendellösung interference effect occurring simultaneously for the broad incident wavelength spectrum of a very-cold neutron beam in the periodic potential of holographic nanostructures.

WED03

14:45-15:15

Colloidal Crystallization Studied by In-situ Synchrotron SAXS and Computer Simulations

Rainer T. Lechner (1)

Max Burian (2), Carina Karner (3), Heinz Amenitsch (2), Maksym Yarema (4), Wolfgang Heiss (5), Christoph Dellago (3), Oskar Paris (1)

(1) Institut für Physik, Montanuniversität Leoben, Leoben, AUT (2) Institute of Inorganic Chemistry, TU Graz, Graz, AUT (3) Faculty of Physics, University of Vienna, Vienna, AUT (4) D-ITET, ETH Zürich, Zürich, SUI (5) Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, GER

Colloidal supercrystals using designed nanocrystals (NCs) as artificial atoms offer the opportunity for realising solids with tailored properties [1]. The self-assembly of colloidal crystals is not only influenced by the NC-size, but also by the shape of the individual NC [2]. We studied by in-situ SAXS the colloidal crystallization by diffusion of a non-solvent into the colloidal dispersion of faceted Bi NCs with around 22 nm size [3]. The SAXS patterns of the NC ensembles were recorded below the NC-solvent/non-solvent interface at the SAXS beamline at ELETTRA.

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Hence, we could follow the crystallization process as a function of the non-solvent concentration. Furthermore, by measuring at different positions below the interface the solvent/non-solvent gradient could be varied and thus its influence on the crystallisation process studied. Many sharp Bragg peaks in the 2D reciprocal space map proved the formation of well-ordered superlattice structures at the capillary wall. The 2D peak patterns can be indexed using a single fcc crystal structure with a lattice of around 24 nm. The crystallite size and the orientation of these supercrystals with respect to the capillary wall, however, differ for different growth speeds: Close to the interface smaller crystallites with hcp stacking faults and a fixed orientation to the glass wall are found, whereas far away from the interface random orientated 3D supercrystals with micrometer size are detected. To test, if this experimentally obtained supercrystals structure is related to the equilibrium superstructure of our densely packed faceted Bi-NCs we theoretically model the crystallization using Monte Carlo simulations [2,4].

As an input we need the exact 3D shape of the individual Bi NCs. For obtaining this shape we developed a new method to retrieve the mean particle shape of slightly polydisperse nanoparticles by advanced SAXS analysis methods [5]. The resulting shape deviates significantly from a sphere and can be described by a strongly faceted oblate ellipsoid related to the rhombohedral crystal structure of Bi. This resultant mean shape was used for the theoretical modelling of the crystallisation.

We found that the simulated and experimental derived structure factors match very well. We could not clearly determine from the experimental diffraction pattern, if the Bi super-crystallites only exhibit positional or also orientational ordering parallel to their surface facets [2]. The simulations, however, show a long range positional ordering that lacks orientational ordering at intermediate packing fractions, rendering it a plastic crystal. At higher packing fractions, we additionally observe the emergence of a local orientational ordering parallel to the Bi surface facets that slowly overtakes the whole system [4]. Thus we are able to link the supercrystal structure via the NC-shape to the atomic Bi crystal structure.

[1] M. V. Kovalenko, et al., W. Heiss, ACS Nano 9 (2015)

[2] A.P. Gantapara et al., M. Dijkstra, PRL 111 (2013)

[3] M. Yarema, et al., W. Heiss, JACS 132 (2010)

[4] M. Burian, C. Karner, R.T. Lechner, to be submitted

[5] M. Burian, et al., R.T. Lechner, J. Appl. Cryst. 48 (2015)

WED04

15:45-16:00

Fluctuating Charge Order: A Universal Phenomenon in Unconventional Superconductivity.

Erminald Bertel

Alexander Menzel

Institute of Physical Chemistry, University of Innsbruck, Innsbruck, AUT

Unconventional superconductors are characterized by various competing ordering phenomena in the normal state, such as antiferromagnetism, charge order, orbital order or nematicity. According to a widespread view, antiferromagnetic fluctuations are the dominant ordering phenomenon in Cuprates and Fe based superconductors and are responsible for electron pairing. In contrast, charge order is believed to be subdominant and to compete with superconductivity. Investigations of anomalous surface phase transitions and their relation to surface ordering phenomena observed in 122 Iron Arsenides led us to postulating the presence of fluctuating charge order in $(0,\pi)$ direction in these compounds[1]. However, the model band structure, on which theoretical studies of Fe based superconductors are generally based, did not support charge ordering in that direction. In contrast, recent angle-resolved photoemission spectroscopy (ARPES) studies reveal a more complex pattern of the Fermi surface topology and indicate strong quasi-particle scattering in the $(0,\pi)$ direction [2]. Moreover, recent experiments on electron doped FeSe superconducting films [3] strongly support the existence of a pairing mechanism independent from antiferromagnetic fluctuations and related to charge correlations in $(0,\pi)$ direction.

Independently, incommensurate charge order in the Cu-O bond direction, i.e. at 45° off the AF spin density wave vector, has been found recently in a variety of cuprates. Refined multiorbital model calculations [4] support the existence of such charge correlations and an alternative pairing mechanism based on charge density wave (CDW) fluctuations near a CDW quantum critical point has been proposed [5]. This highlights striking parallels between the Fe based and the cuprate superconductors.

Here we argue [6] that fluctuating charge order in $(0,\pi)$ direction is a general feature shared by the Cuprates and the Fe based

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superconductors alike. Quantum fluctuations of charge order provide an alternative to spin fluctuations as a mechanism of electron pairing in unconventional superconductors. As a consequence, we suggest to tune charge-ordered materials to a quantum critical point, where charge order disappears and to examine them for unconventional superconductivity.

1. Cordin, M.; Amann, P.; Menzel, A.; Bertel, E.; Baranov, M.; Diehl, S.; Redinger, J.; Franchini, C. Comment on "Cleavage surface of the Ba-Fe_{2-x}CoxAs₂ and Fe_ySe_{1-x}Tex superconductors: A combined STM plus LEED study". *Physical Review B* 2012, 86, 167401.
2. Kordyuk, A.A.; Zabolotnyy, V.B.; Evtushinsky, D.V.; Yaresko, A.N.; Büchner, B.; Borisenko, S.V. Electronic band structure of ferro-pnictide superconductors from ARPES experiment. *Journal of Superconductivity and Novel Magnetism* 2013, 26, 2837-2841.
3. Song, C.-L.; Zhang, H.-M.; Zhong, Y.; Hu, X.-P.; Ji, S.-H.; Wang, L.; He, K.; Ma, X.-C.; Xue, Q.-K. Observation of double-dome superconductivity in potassium-doped FeSe thin films. *Physical Review Letters* 2016, 116, 157001.
4. Atkinson, W.A.; Kampf, A.P.; Bulut, S. Charge order in the pseudogap phase of cuprate superconductors. *New Journal of Physics* 2015, 17, 013025.
5. Wang, Y.; Chubukov, A.V. Enhancement of superconductivity at the onset of charge-density-wave order in a metal. *Physical Review B* 2015, 92, 125108.
6. Bertel, E.; Menzel, A. Fluctuating charge order: A universal phenomenon in unconventional superconductivity? *Symmetry* 2016, submitted.

WED05

16:00-16:15

Manifestation of many-body interactions in the integer quantum Hall effect regime

Josef Oswald (1)

Rudolf Römer (2)

(1) Montanuniversität Leoben, Leoben, AUT (2) University of Warwick, Department of Physics, Warwick, GBR

The challenge of modelling experimental investigations of the QHE regime is the requirement of a link between the many particle Fermi sea (usually modelled as a stationary many particle ground state) and the experimentally injected non-equilibrium [1]. Our model consists of two modules: One addresses the stationary many particle Fermi sea on the basis of a self-consistent numerical Hartree-Fock approach [2] and the other module addresses the non-equilibrium electron transport in the integer quantum Hall effect regime [3]. The latter is based on a transfer matrix approach within a network model for the lateral distribution of the non-equilibrium electrochemical potential that is injected by contacts in the various experimental setups. The combination of the two modules allows us to simulate directly the non-equilibrium potential distributions at arbitrarily arranged contact configurations, including native and artificial in-homogeneity. The associated resistances and conductance's need to be calculated only in a post processing step like it is also the case in real experiments. There are two possible mechanisms for the communication between the many particle system (Hartree-Fock module) and the non-equilibrium network transport module (NNM): One is to communicate with the NNM via coulomb effects and the other is communication via the local filling factors. For the high carrier density regime like addressed in this presentation the latter turns out to be the more general one. In this regime many particle effects like the filling factor dependent exchange enhanced g-factor dominate over pure electrostatic effects like native disorder potential fluctuations. Our results exhibit a strong tendency of the electron system to avoid the simultaneous existence of partly filled spin-up and spin-down Landau levels (LLs), which can be understood as a driving force for many particle effects like the exchange enhanced g-factor. Partly filled LLs appear as a mixture of coexisting regions of full and empty LLs. We obtain edge stripes with approximately constant filling factor close to half filling at the boundaries between the regions of full and empty LLs, which we explain in terms of the oscillatory g-factor enhancement as a function of the filling factor, which locally varies across the stripes. All in all the many particle interactions follow a behavior as it would result from applying Hund's rule and the screening of the disorder and edge potential appears widely suppressed as compared to screening based on a Thomas-Fermi approximation like used by D.B. Chlovskii et al, which up now is used as the state of the art model for screening in the IQHE regime [4]. However, there exist recent scanning gate investigations of

compressible stripes [5] which indicate that the Thomas-Fermi approach may overestimate the screening behavior in this regime.

1. J. Oswald; Linking non-equilibrium Electron Transport with the Many-Particle Fermi Sea in the Quantum Hall Regime, Chapter in Research Advances in Quantum Dynamics, Ed. Paul Bracken, Univ. Texas, ISBN 978-953-51-4735-0, in print

2. C. Sohrmann, J. Oswald, R.A. Römer R.A., Lecture Notes in Physics 762, pp. 163-193 (2009)

3. J.Oswald, M. Oswald, JOURNAL OF PHYSICS C 18 - 7, R101-R138 (2006)

4. D.B. Chlovskii, B.I. Shklovskii, L.I. Glatzman, Phys.Rev. B46, 4026 (1992)

5. N. Pascher, F. Timpu, C. Rossler, C. Reichl, T. Ihn, K. Ensslin, C. Reichl, W. Wegscheider, Phys. Rev. X 4, 011014 (2014)

WED06

16:15-16:30**Experimental determination of spin Hall angle in wurtzite n-GaN:Si**

Rajdeep Adhikari

Margherita Matzer, Aitana Tarazaga Martin-Luengo, Alberta Bonanni

Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, AUT

The generation of pure spin currents in functional semiconductors is a fundamental requirement for the implementation in the next generation of spin-based devices. Besides being strategic material systems for state-of-the-art optoelectronics and high power electronics, III-nitride semiconductors like GaN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ doped with magnetic elements have been widely studied as dilute magnetic semiconductors [1-5].

Moreover, with a non-negligible Rashba spin-orbit coupling parameter of $(4.5 \pm 1.0) \text{ meV} \cdot \text{\AA}$ [6] and long spin relaxation times, n-GaN:Si is an outstanding workbench for the generation and manipulation of pure spin currents.

We report on the generation of pure spin currents in degenerately doped wurtzite n-GaN:Si using an adiabatic spin pumping technique at room temperature and estimate the spin Hall angle θ_{SH} for this Rashba semiconductor. A Py/n-GaN:Si bilayer system is driven to a ferromagnetic resonance condition and the voltage from an induced charge emf,

due to the interplay of the direct and inverse spin Hall effects, have been measured simultaneously. The measured voltage is resolved into symmetric and asymmetric components [7] due to spin Hall- and galvanomagnetic-effects. From the fundamental model of spin pumping [8,9], a spin mixing conductance of $(1.38 \times 10^{18}) \text{ m}^{-2}$ for the Py/ n-GaN:Si interface and a spin Hall angle $\theta_{\text{SH}} = 3.03 \times 10^{-3}$ for wz n-GaN:Si are found [10]. The obtained value of θ_{SH} is at least one order of magnitude higher than those obtained for other semiconductors like Si, Ge, ZnO and n-GaAs [7]. We do not observe any spin pumping from an oxidised Py layer on n-GaN:Si or for a Schottky interface, as in the case for Py/u-GaN (undoped) thereby highlighting the quality of the ferromagnet/non-magnet interface. We also demonstrate explicitly the effect of the non-magnetic layer thickness on the nature of the generate emf and discuss the contributions of spurious galvanomagnetic effects, like planar Hall effect (PHE) in the Py, to the measured emf. This work paves the way to the realization of nitride based low power, non-volatile and non-dissipative spin devices e.g. spin batteries [11].

A. Bonanni et al. Phys. Rev. Lett. 101, 135502 (2008). T. Devillers et al. Sci. Rep. 2, 722 (2012) T. Dietl et al. Rev. Mod. Phys. 87, 1311 (2015). R. Adhikari et al. Phys. Rev B 91, 205204 (2015) M. Rovezzi et al. Phys. Rev. B 92, 115308 (2015). W. Stefanowicz et al. Phys. Rev B 89, 205201 (2014). J. Sinova et al. Rev. Mod. Phys. 87, 1213 (2015). Y. Tserkovnyak et al. Phys. Rev. B 66, 224403 (2002). Y. Tserkovnyak et al. Rev. Mod. Phys. 77, 1375 (2005). R. Adhikari et al. arxiv: 1603.06471 (2016). A. Brataas et al. Phys. Rev. B 66, 064404 (2002)

WED07

16:30-16:45

Improving the strength in SPD deformed nanometals using vacancy clusters

Daria Setman

Peter Cengeri, Jelena Horky, Katharina Werbach, Erhard Schafner, Michael Zehetbauer

Faculty of Physics, University of Vienna, Vienna, AUT

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After severe plastic deformation (SPD) metals exhibit markedly enhanced strength levels because of the ultrafine grained structure reached, but due to the nanostructure left in the grain interiors there is still potential for further improvements. Agglomerates of vacancies can lead to a significant increase in strength, even if the vacancies arise from plastic deformation [1]. In this presentation we report on strength investigations of Cu, Ni, and Mg after High Pressure Torsion (HPT) and after subsequent heating. Strength was characterized by microhardness and nanoindentation tests. DSC scans were done in parallel to the strength investigations in order to analyse the HPT-induced defects. All metals reveal vacancy agglomerate-induced strength increases up to 25%. From the dependence of annealing temperature on HPT applied shear strain it is concluded that in Cu and Ni planar vacancy loops form. Recent experiments applying HPT and thermal treatment on Mg-Zn-Ca biomedical alloys revealed hardness increase up to 60%; these can be associated to vacancy agglomeration because analogous effects have been found in samples quenched from high temperatures, and because the hardening of SPD-induced precipitations was found to be far too small to account for this significant hardening effect [2, 3].

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[1] M. Zehetbauer, *Key Eng.Mater.* 97-98, 287 (1994)

[2] J. Horky, A. Ghaffar, A. Grill, S. Pogatscher, B. Mingler, P. J. Uggowitzer, M.J. Zehetbauer; Lecture at the Int.Conf. NanoSPD6, Metz (France), July 2014, also reported in: R. Z. Valiev, Y. Estrin, Z. Horita, T. G. Langdon, M. J. Zehetbauer, Y. T. Zhu *Mater.Res.Lett.* 4, 1-21 (2016)

[3] K. Werbach, Master Thesis, University of Vienna, Austria (2016) (in cooperation with R. Schäublin and J. Löffler, Department of Materials, ETH Zurich, Switzerland)

WED08

16:45-17:00

AFM based dynamic mechanical analysis of viscoelastic properties of cellulose fibers

Caterina Czibula (1)

Christian Ganser (1), Ulrich Hirn (2), Christian Teichert (1)

(1) Institute of Physics, Leoben, AUT (2) Institute for Paper, Pulp and Fiber Technology, Graz, AUT

There are several scanning probe microscopy (SPM) methods providing tools to investigate mechanical properties by measuring the interaction of a sharp probe with the specimen's surface. Probing nanoscale mechanical properties of soft materials with atomic force microscopy (AFM) yields information about the performance of the polymer systems – in this case cellulose fibers as an inhomogeneous and complicated hierarchical system. Furthermore, precise force control in AFM methods can be used to examine rate dependent material's response. Therefore, dynamic mechanical analysis (DMA) which is well-known for polymer characterization was adapted as an AFM method. In DMA, a sinusoidal force is applied to the material and the resulting displacement is measured. Here, force-distance curves were recorded, and during contact a sinusoidal loading for different frequencies was applied. With the phase shift between force and displacement, it is possible to calculate the storage and loss moduli of the material. The bulk behavior of viscoelastic materials is often represented with simple empiric models combining springs and dash pots, which are used at the continuum scale. Simple models include the Maxwell and the Kelvin-Voigt model. However, to describe real materials properly the standard linear solid (SLS) or the Wiechert model are more often used. These models describe material properties like viscosity. Here, it was tried to apply some of the different viscoelastic models to cellulose fibers and compare them with each other.

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WED09

17:00-17:15

Electro-osmotic flow in bicomponent fluid

Andrei Bazarenko

Marcello Sega

Faculty of Physics, University of Vienna, Vienna, AUT

The electro-osmotic flow and the Droplet Electrophoresis are two phenomena relying on the action of an external electric field on solvated counter ions, which are used to transport fluids in microfluidic devices. Interestingly, both phenomena can be seen as two extreme cases of the same physical model, where the solvation free energy of the counter ions is the control parameter of a continuous transition between the electro-osmotic and the electrophoretic cases. In this study we investigate numerically, how several physical properties change during this transition, by solving the coupled equations of motion of the counter ions in interaction with a continuous model of the flow. The system is modelled by coupling the Langevin equation of motion of off-lattice, point-like counter ions (interacting through the full, long range electrostatics) with an on-lattice description of a bicomponent fluid, simulated using the Shan-Chen model. The presence of explicit ions allows us to go beyond the simple Poisson-Boltzmann approximations, and investigate a variety of flow regimes.

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WED10

13:45-14:00

Development of the V0+ detector of the Fast Interaction Trigger (FIT) for the Upgrade of the ALICE Detector

Mohamed Awadein (1)

A. Lanz (1), J. Zmeskal (1), K. Suzuki (1), A. Menchaca-Rocha (2), D. Serebryakov (3), G. Ahmed (4), L. Gruber (1), M. Weber (1), R. Alfaro-Molina (2), T. Karavicheva (4), V. Grabski (2), W.H. Trzaska (5), M. Slupecki (5)

(1) Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT (2) Universidad Nacional Autonoma de Mexico, Mexico City, MEX (3) MEPH, Moscow, RUS (4) Azhar University in Cairo, Cairo, EGY (5) Institute for Nuclear Research, Moscow, RUS (5) University of Jyväskylä, Jyväskylä, FIN

ALICE (A Large Ion Collider Experiment) is one of four large experiments of the LHC. ALICE is dedicated to the study of strongly interacting matter in heavy ion collisions. In its present configuration, there are two independent sub detectors (T0 and V0), that provide minimum bias trigger, multiplicity trigger, beam-gas event rejection, collision time for the Time of Flight detector (TOF), on line multiplicity and event plane determination.

In its proposed future version, ALICE integrates upgraded T0+ and V0+ into a single system, the Fast Interaction Trigger (FIT). V0+ is composed of a disk of plastic scintillator segments and is used to estimate the centrality of the collision by summing up the energy deposited in the disk. The Stefan-Meyer-Institut is mostly contributing to the FIT project with a silicon photomultiplier solution for the V0+ photo-sensor and we will present the results from the test of our prototype at CERN PS facility at the last beam time in June 2016. The current prototype consists of a 10x10 cm ² EJ-228 scintillator placed down-stream from a Cherenkov telescope, composed of two quartz crystals. The light output generated in the scintillator is collected using an optical fiber matrix, uniformly

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distributed over the scintillator's output face. The other end of the fibers is bundled together and coupled to a 30:9 mm reducing light guide, read by a 4 mm 2 square Hamamatsu 6x6 SiPMT matrix, having no pre-amplified output. The V0+ detector shall be located in a radiation harsh environment. It is required to have a time resolution <200 ps, a high dynamic range, and to provide a linear output. It must also be able to operate in a 25 ns bunch-crossing mode.

WED11

14:00-14:15

The First-Level Trigger of the CMS Experiment at the LHC

Manfred Jeitler

HEPHY, Austrian Academy of Sciences, Vienna, AUT

Several Austrian physics institutes are active at CERN. The Institute of High Energy Physics of the Austrian Academy of Sciences in Vienna (HEPHY) is playing an important role in the CMS experiment at CERN's LHC collider, above all in the trigger electronics, the Silicon tracking detector and in physics data analysis.

The First-Level Trigger of the CMS Experiment serves to reduce the event rate from 40 MHz - the rate at which proton bunches collide in the LHC - to 100 kHz, the rate at which data can be read out from the CMS detector. These data are then forwarded to the computer farm of the High-Level Trigger, which further reduces the event rate to below 1 kHz. The Trigger system has been operating since the startup of the LHC and has been a key component in discoveries such as that of a Higgs boson. To improve the trigger's performance and reliability, the system was completely rebuilt after LHC's Run I. Electronics was redesigned to switch from the old VME crate standard to the new microTCA system (TCA stands for Telecommunications Architecture). In many parts of the digital trigger electronics, reprogrammable integrated circuits are used, so-called "Field Programmable Gate Arrays" (FPGAs).

The Global Trigger designed by HEPHY is the final decision stage of the First-Level Trigger. The upgraded system is based on the most recent and powerful FPGA, the "Virtex-7" and uses its resources to integrate more and more complex calculations traditionally limited to computers into the upstream domain of digital electronics. The Global Trigger can

make selections based on topological conditions including muons, electrons, photons, jets, energy sums and missing transverse momentum. This allows us to make full use of the high collision rates experiments have to cope with at the present LHC center-of-mass energy of 13 TeV and the high luminosity achieved by the collider. In addition to the Global Trigger, HEPHY has also designed important parts in the muon trigger chain, the “Barrel Muon Track Finder” and the “Global Muon Trigger”.

The presentation will cover the design and physics potential of the CMS trigger and the experience from the first year of data taking with the upgraded system, with special emphasis put on the systems designed by Austria.

WED12

14:15-14:30

Module concepts and status of sensor qualification for the CMS tracker phase 2 upgrade

Johannes Grossmann

HEPHY, Austrian Academy of Sciences, Vienna, AUT

During the high luminosity era of LHC a luminosity of $5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ and an integrated luminosity of 3000 fb^{-1} will be delivered. In order to achieve the physics goals at 140 collisions per bunch crossing tracking algorithms require a higher granularity as in the current CMS Tracker. Existing bandwidth limitations require a reduction of the amount of data at module level. Therefore the a major detector upgrade is necessary. New modules have binary readout, on-chip p_t discrimination and capabilities to provide track finding data at 40MHz to the L1-trigger. The CMS collaboration has undertaken R&D effort to develop new planar sensors for the pixel-strip (PS) module, which has to withstand $1 \times 10^{15} \text{ cm}^{-2}$ 1MeV neutron equivalent fluence in the innermost layer of the tracker. The module is composed of a strip sensor and a macro pixel sensor with $100 \mu\text{m} \times 1.5\text{mm}$ pixel size. A small prototype ROC for the PS-pixel sensor was developed and a first subassembly was built. The chip is bump-bonded to the assembly and noise studies of the un-connected bumps are made, which may be used to qualify assemblies during the production process. In this talk the status and progress of

the sensor qualification and the module concept for the CMS Tracker upgrade will be presented.

WED13

14:30-14:45

PET range verification of ion beam therapy at MedAustron

Heide Rohling (1)

Albert Hirtl (1), Marta Mumot (2), Lembit Sihver (1,2), Markus Stock (2)

(1) Atominstytut, TU Wien, Vienna, AUT (2) EBG MedAustron GmbH, Wiener Neustadt, AUT

At the MedAustron facility in Wiener Neustadt cancer patients will be treated with proton beams and carbon ion beams, with proton therapy planned to start this year. Carbon ion beams have a high biological effectiveness and facilitate the treatment of hypoxic tumors. For both, proton and carbon ion beams, the therapeutic irradiation is advantageous over conventional treatment with photons or electrons regarding the precision of the dose delivery. This is due to the characteristic depth dose profile of protons and other light ions in matter, exhibiting a maximum close to the end of the range of these particles at the so-called Bragg peak. Therefore, for deep-seated tumors, normal tissue can be spared better compared to conventional irradiation. Especially, the sharp decline of the depth dose profile behind the Bragg peak allows the treatment of tumors which are in vicinity of organs at risk. But this also bears the risk that in case of deviations from the treatment plan, e.g., anatomical changes, range shifts occur that can lead to overdosage in the organs at risk or underdosage in the tumor. In order to ensure the best clinical outcome of the therapeutic irradiation with ion beams, a non-invasive in-vivo range verification of ion beam therapy is highly desired.

A feasible method for range monitoring is positron emission tomography (PET). During the irradiation of human tissue with protons and other ions, β^+ -emitting isotopes are produced in nuclear reactions as a by-product of the treatment. The resulting annihilation photons are detected and the distribution of the positions of annihilations can be deduced. In order to evaluate the PET measurement, the established method is to predict the β^+ -activity based on the treatment plan by means of simulations. These simulations include in the optimal case

all physical processes from the production of the β^+ -emitting isotopes to the detection of the annihilation photons with the PET camera. The predicted and the measured data are in the best case reconstructed with the same algorithm and compared using semi-automated routines. Despite limitations of this method, such as the low activity compared to PET for nuclear medicine, or the washout due to blood flow, PET has been applied successfully at several particle therapy centers for range monitoring, during (in-beam PET) or directly after the treatment (off-line PET). At MedAustron, a Philips Gemini Big Bore PET/CT exclusively dedicated to off-line PET is available close to the treatment room. We present our approaches for the development of the software framework required for the PET range verification work flow, i.e., the components for the simulation of the β^+ -activity and the modeling of the detector using the Geant4-based simulation tool GATE. Furthermore, plans for first tests of the PET work flow with activated plastic targets will be shown.

WED14

14:45-15:00

The CLIC Vertex Detector

Florian Pitters

CERN, Geneva, SUI

CLIC is a concept for a future linear collider that would provide e+e- collisions at a centre-of-mass energy of up to 3 TeV. The physics aims require a detector system with excellent jet energy and track momentum resolution, highly efficient flavour-tagging and lepton identification capabilities, full geometrical coverage extending to low polar angles and effective rejection of beam-induced background.

For the vertex detector, this translates to a single-point spatial resolution below 3 microns, extremely low material budget and a time resolution in the order of nanoseconds. A concept based on hybrid planar pixel-detector technology is under development. It consists of fast, low-power and small-pitch readout ASICs implemented in 65 nm CMOS technology (CLICpix) coupled to ultra-thin sensors via low-mass interconnections. Power pulsing capabilities will allow for forced gas flow cooling.

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This talk provides an overview of the requirements and design optimisations for the CLIC vertex detector concept as well as recent R&D activities on detector technologies.

WED15

15:00-15:15

Timing resolution performance of the PANDA SciTil detector using Silicon Photomultiplier (SiPM)

Marius Constantin Chirita Mihaila (1)

Lukas Gruber (1), Ken Suzuki (1), Merlin Böhm (2), Albert Lehmann (2), Dominik Steinschaden (1), Gamal Ahmed (3)

(1) Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT (2) University of Erlangen-Nuremberg, Erlangen, GER (3) Al-Azhar University, Physics Department, Cairo, EGY

The PANDA experiment at FAIR situated in Darmstadt, Germany will use proton-antiproton annihilation with a momentum range from 1.5 GeV/c to 15 GeV/c for strong interaction studies. The detector is currently under construction. It will be in operation in 2022-. In order to identify the charged particles accurately and differentiate between subsequent events the detector will need several advanced particle identification systems.

We are working on the development of a SciTil (Scintillator Tile Hodoscope) detector, which is located in the central region (20° -140°) and covers ~5.7 m² area. It is constituted of 1920 scintillator tiles, each of which has a dimension of 90x30x5 mm³, readout by Silicon Photomultipliers (SiPM). The SciTil detector will be capable of providing a fast and highly accurate event timing. The requirements for this detector are an intrinsic time resolution below $\sigma = 100$ ps and a geometry which fits along 2 cm in radial direction.

Development of a single tile is in a final phase. After optimizing scintillator material, sensor, wrapping etc., we achieved the best time resolution of $\sigma \sim 50$ ps with 4 Hamamatsu SiPMs S13360-3050-PE connected in series. In this presentation, the final design and its performance of a single tile will be presented.

WED16

15:45-16:00

Status and Plans of the CRESST Experiment

Cenk Turkoglu

HEPHY, Austrian Academy of Sciences, Vienna, AUT

It is known from several astronomical observations that dark matter contributes 27 % to the overall energy density of our universe but its nature has not been understood so far. The CRESST experiment aims to directly detect dark matter particle elastically scattering off nuclei. The CRESST-II detector modules are based on CaWO₄ crystals which are operated at mK temperatures. The nuclear recoil energy thresholds for the CRESST-II detectors Lise and TUM40 are 0.3 keV and 0.6 keV, respectively. Low energy thresholds make CRESST ideally suited for the detection of low-mass dark matter particles. Further increase in sensitivity is expected with CRESST-III detectors featuring a threshold of 0.1 keV. In this talk, we will present our results on the search for the dark matter obtained with the detector modules Lise and TUM40 of CRESST-II. We will discuss the status of CRESST-III Phase 1 which started taking data this year. In addition to the low threshold, radio purity of the crystals is another important factor for the detection of dark matter particles. To acquire a detailed understanding of the backgrounds measured by the detectors, a Geant4 simulation of the electromagnetic backgrounds was carried out for the TUM40 detector module. The simulation includes backgrounds coming both from inside the crystal and from outside. The information taken from the background simulation will be used in the construction and purification of the detectors for the second phase of the CRESST-III experiment. Additionally, an outlook for the upgrade of the readout electronics of CRESST-III Phase 2 will be discussed.

WED17

16:00-16:15

Probing Gravity with Ultracold Neutrons in the qBounce Experiment

Mario Pitschmann

TU Wien, Vienna, AUT

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The qBounce experiment will be presented: ultracold neutrons fall in the gravity potential of the earth and are reflected from a mirror. As a bound quantum system, the neutrons have discrete energy eigenstates and are found in a coherent superposition of particular levels. The lowest discrete states are in the range of several pico-eVs. This opens the way to probe theories of gravitational interaction and dark energy.

WED18

16:15-16:30

Identifying the sources of gravitational wave signals

Sascha Husa

University of the Balearic Islands, Palma, ESP

The discovery of a gravitational wave signal of cosmic origin with the LIGO detectors in September 2015 has initiated a new era in astronomy and fundamental physics. This talk will focus on how the properties of the sources of gravitational wave events are inferred from comparing observational data to solutions of the Einstein equations, and how such solutions are modelled by synthesising information from perturbative treatments of the Einstein equations, and from non-perturbative numerical solutions. I will summarise what has been learned so far from gravitational wave observations about astrophysics, and report on tests of general relativity in the strong field regime. To conclude, I will discuss the future of the field, and how gravitational wave science relates to other areas in physics.

WED19

16:30-16:45

Dissipative Losses in Self-Interacting Dark Matter Collisions

Lukas Semmelrock

HEPHY, Austrian Academy of Sciences, Vienna, AUT

Dark matter self-interactions are frequently put forward in the explanation of small structure problems in the universe. They could have important implications on the formation and evolution of structures,

from dwarf galaxies to large galaxy clusters. I will present the effects of bremsstrahlung in self-interacting dark matter collisions on structure formation by studying four different dark matter models perturbatively in a non-relativistic and non-degenerate limit. To analyze the effect of radiative cooling on structure formation, I compare the cooling time of a gas of dark matter particles to the elastic scattering time scale, the Hubble time and the gravitational timescale. Results show that for a fiducial dark matter density of 1 GeV/cm^3 , which is approximately the dark matter density in our local group, the effects of radiative cooling on structure formation are negligible, considering observational constraints on the elastic self-scattering cross section. However, in regions of the universe where the dark matter density is a few orders of magnitude higher, parameters can be found such that cooling can influence structure formation while satisfying the observational constraints.

WED20

16:45-17:00

CPT symmetry and gravity tests with antihydrogen

Chloé Malbrunot (1,2)

(1) CERN, Genève, SUI (2) Stefan Meyer Institute, Austrian Academy of Sciences, Wien, AUT

On behalf of the AEGIS and ASACUSA collaborations A growing number of collaborations are performing experiments at the CERN Antiproton Decelerator (AD), the only available facility providing slow antiprotons suitable for precision measurements with anti-atoms. The majority of these experiments are forming antihydrogen atoms with the main goal of probing the atomic transitions which have been measured in hydrogen to a remarkable precision. The precise comparison between the hydrogen and antihydrogen transitions has indeed the potential to provide one of the most sensitive tests of CPT symmetry. More recently, experiments have begun to employ antihydrogen atoms to test the validity of the Weak Equivalent Principle on antimatter by measuring the fall of these anti-atoms in the Earth's gravitational field.

I will focus my talk on the recent developments of the ASACUSA-CUSP and AEGIS experiments. AEGIS plans on performing a direct measurement of the acceleration of cold antihydrogen atoms in the Earth gravitational field with a precision of 1 to 10% in the first experimental

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phase while the ASACUSA-CUSP experiment aims at measuring the ground-state hyperfine splitting of antihydrogen to the ppm level using an atomic spectroscopy beamline.

After shortly describing the experimental setups and discussing their respective sensitivities, I will highlight the latest developments and the upcoming experimental challenges towards the first CPT and gravity tests with antihydrogen.

WED21

17:00-17:15

How to break a no-go theorem in Dark Matter direct detection

Josef Pradler

HEPHY, Austrian Academy of Sciences, Vienna, AUT

The direct detection of Dark Matter particles with mass below the GeV-scale is hampered by soft nuclear recoil energies and finite detector thresholds. For a given maximum relative velocity, the kinematics of elastic Dark Matter nucleus scattering sets a principal limit on detectability. Here we propose to bypass the kinematic limitations by considering inelastic channels in the nuclear recoil. Our proposed method allows to probe MeV-scale Dark Matter in the plane of Dark Matter mass and cross section with nucleons. In situations where a Dark Matter-electron coupling is absent, our proposal constitutes a path to probe low-mass Dark Matter with current state-of-the-art detectors.

THEO

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13:45-14:00**Three dimensional Black Holes, Microstates and the Heisenberg Algebra**Wout Merbis*Institute for Theoretical Physics, TU Wien, Vienna, AUT*

Lower dimensional theories of gravity have been a fruitful arena to address conceptual questions in quantum gravity. Especially the presence of black holes in 2+1 dimensional gravity provides an interesting window into the nature of black hole statistical mechanics and thermodynamics. The topological nature of three dimensional gravity ensures that dynamical degrees of freedom arise only on the boundary of the manifold, after choosing suitable boundary conditions. We will propose a new set of boundary conditions which accommodates space-times with horizons (e.g. black holes) and show that the relevant degrees of freedom for these space-times are governed by a simple Abelian current algebra. This algebra is essentially equivalent to the Heisenberg algebra. The associated conserved charges can then be interpreted as „soft hair“ on the horizon, in the sense that they are strictly zero-energy excitations. Finally, we address the relation between these soft horizon charges and the conformal generators at asymptotic infinity, black hole microstates and generalizations to cosmological horizons.

WED23

14:00-14:15**Three dimensional gravity**Friedrich Schöller*TU Wien, Vienna, AUT*

We live in a Universe with four observable space-time dimensions. Quantum mechanics describes to incredible precision the small scale of the Universe. Einstein's theory of gravity teaches us about the large scale structure of space-time. Combining these two theories and constructing a quantum theory of gravity is one of the great outstanding tasks of theoretical physics. While there are many open conceptual problems, there are also many technical ones. Some of which can be removed by reducing the number of space-time dimensions. I talk about aspects of the approach to quantum gravity in three dimensions.

WED24

14:15-14:30**The Einstein flow on surfaces**David Miro Fajman*Faculty of Physics, University of Vienna, Vienna, AUT*

Determining the global geometric structure of cosmological spacetimes is one of the central problems in mathematical cosmology. A particular aspect in this study concerns the relation between the spatial topology of a spacetime and the long-time behavior of the Einstein flow. The major competing scenarios are spacetimes that eternally expand vs. those ones that recollapse, i.e. contain both a big-bang and a big-crunch singularity. A toy model to study this problem is provided by 2+1-gravity, where the spatial topology is restricted to spheres, tori and hyperbolic surfaces. As 2+1-gravity is a well-studied system in particular in the context of quantum gravity it is relevant for its own sake to determine the global structure of cosmological models in that system. Surprisingly, models of this type have to our knowledge rarely been studied. A major reason for this may be that, considering the vacuum Einstein-flow, only few solutions exist. In this talk we show that this is drastically changed if the non-vacuum Einstein-flow (for instance the Einstein-Vlasov system) is considered -- modeling ensembles of self-gravitating collisionless particles. If non-vacuum initial data is considered, large classes of 2+1-dimensional cosmological spacetimes exist. These spacetimes show a variety of different global structures such as recollapsing models as well as eternally expanding models -- depending on the spatial topology and the mass of particles involved in the system. Moreover,

these solutions have additional desirable features, which we will explore in the talk. As this class of spacetimes is essentially unknown up until now it is likely to provide substantial insight into the long-time behavior of the Einstein-flow.

WED25

14:30-14:45

News from low regularity GR

Roland Steinbauer

Faculty of Mathematics, University of Vienna, Vienna, AUT

The motivation for the study of spacetimes where the metric is of low regularity is twofold. First, many physically reasonable models necessitate the matter variables to be discontinuous and so the the field equations force the metric to be below C^2 . Second, the recent existence theory for the Einstein equations typically provide metrics which are merely continuous on the time slices.

In this talk we report on recent progress in the study of spacetimes of low regularity, focussing on the regularity classes $C^{0,1}$ and $C^{1,1}$, i.e., locally Lipschitz continuous metrics and metrics with locally Lipschitz continuous first order derivatives. In the first case we present results on the existence, regularity and completeness of geodesics [S:14] and discuss some applications to impulsive gravitational waves (e.g. [PSSS:15]). In the second case we discuss recent advances in causality theory and, in particular, the recent proofs of singularity theorems in $C^{1,1}$ ([KSSV:15, KSV:15]).

[S:14] R. Steinbauer, Every Lipschitz metric has C^1 -geodesics, Class. Quant. Grav. 31, 2014.

[PSSS:15] J. Podolsky, C. Sämann, R. Steinbauer, R. Svarc, The global existence, uniqueness and C^1 -regularity of geodesics in nonexpanding impulsive gravitational waves. Class. Quant. Grav. 32, 2015.

[KSSV:15] M. Kunzinger, R. Steinbauer, M. Stojkovic, J. Vickers, Hawking's singularity theorem for $C^{1,1}$ -metrics. Class. Quant. Grav. 32, 2015.

[KSV:15] M. Kunzinger, R. Steinbauer, J. Vickers. The Penrose singularity theorem in regularity $C^{1,1}$. Class. Quant. Grav. 32, 2015.

WED26

14:45-15:00**On Lorentzian causality theory in low regularity**Clemens Sämann*Faculty of Mathematics, University of Vienna, Vienna, AUT*

The solution theory for Einstein's equations and physically relevant models of spacetimes (e.g. matched spacetimes, shock and impulsive waves, conical singularities, etc.) lead to metrics of regularity below $C^1(1,1)$. This class (i.e., the first derivative of the metric exists and is Lipschitz continuous) is the largest class, where the bulk of classical Lorentzian geometry remains valid. Consequently, developing Lorentzian geometry and causality with metrics below this threshold is a desirable goal for working with spacetimes of low regularity.

In this talk we will discuss causality theory for spacetimes with continuous metrics. In particular, we discuss different equivalent notions of global hyperbolicity, the causal ladder and maximal causal curves. In fact, we show that global hyperbolicity implies the existence of maximal causal curves between any two causally related points (the Avez-Seifert theorem).

Surprisingly, these maximal causal curves need not be piecewise C^1 . In [LY] it was proven that in a Riemannian manifold with α -Hölder continuous metric, geodesics (minimizing curves) are $C^1(1,\beta)$, where $\beta = \alpha / (2-\alpha)$.

Thus an analog of [LY] cannot hold in Lorentzian geometry. This is in part joint work with Michael Kunzinger.

[KS] Kunzinger M., Sämann C., Regularity of maximal curves, in preparation

[LY] Lytchak A., Yaman A., On Hölder continuous Riemannian and Finsler metrics, Trans. Amer. Math. Soc. 358 7 2006

[S] Sämann C., Global Hyperbolicity for Spacetimes with Continuous Metrics, Ann. Henri Poincaré 17 (6) 1429-1455 2016

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15:00-15:15

Relativistic, Nonlinear Effects on Large Scales

Hedda Gressel

ICG, University of Portsmouth, Portsmouth, GBR

The universe is homogeneous and isotropic on large enough scales. However, going to smaller scales, we find inhomogeneities such as galaxy cluster, voids, etc., forming today's observable large scale structure. It is assumed that these structures are seeded by small inhomogeneities in the very early universe. We treat the inhomogeneities as small deviations (at early times or large scales) from the Friedmann-Lemaitre-Robertson-Walker (FLRW) model using perturbation theory.

Standard n-body simulations use Newtonian gravitational dynamics on an expanding background instead of the relativistic description. At first order, the Newtonian approach seems to be sufficient for results of significant value. However, at second order, relativistic contributions arise. With increasing precision of surveys higher order effects become measurable and, thus, play an important role in today's cosmology.

In Newtonian gravity, the source and field are linearly related via the Poisson equation. Yet in General Relativity (GR), the field equations are non-linear. Thus, beyond linear order, we obtain additional effects such as non-Gaussian contributions in the matter density field even with Gaussian initial conditions.

In this talk, I will discuss this effect and will present third and fourth order solutions of the density contrast with non-Gaussian contributions within the approximation of a gradient expansion.

WED28

15:45-16:00

Soft lepton number violation in multi-Higgs doublet seesaw models

Elke Aeikens

Walter Grimus

Faculty of Physics, University of Vienna, Vienna, AUT

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Extensions of the Standard Model with right-handed neutrinos ν_R in the framework of a seesaw mechanism are popular to explain the smallness of the neutrino masses. In our model, we additionally allow an arbitrary number of Higgs doublets. Since such models have flavour-changing neutral-scalar interactions (FCNIs) at tree level, we impose conservation of the family lepton numbers L_α ($\alpha = e, \mu, \tau$) in the Yukawa interactions whereas the Majorana terms violate the L_α .

An interesting feature of this model is that FCNI processes are finite at one-loop level and amplitudes like $\mu \rightarrow e^- e^+ e^-$ containing Higgs-scalar exchanging subprocess, in contrast e.g. to $\mu \rightarrow e\gamma$, do not vanish when the ν_R -mass scale m_R becomes infinitely large. Therefore, they could be testable in future experiments. Furthermore, processes provide bounds on Yukawa couplings and the seesaw scale m_R .

WED29

16:00-16:15**One-loop corrections to fermion masses and flavour symmetries**Maximilian Löschner

Walter Grimus

Faculty of Physics, University of Vienna, Vienna, AUT

Extensions of the Standard Model which explain non-vanishing neutrino masses and some of the peculiar features of the lepton mixing matrix by flavour symmetries always lead to a proliferation of scalars in the model. Then, the relation between Yukawa couplings and fermions in general involves several vacuum expectation values. It is therefore expedient to devise a renormalization procedure which is adapted to this situation. We will present first results of an ongoing PhD project addressing this subject. The idea is to calculate one-loop corrections to fermion masses in a toy model featuring an arbitrary number of Majorana or Dirac fermions and scalar fields, testing the stability of tree level predictions for masses and mixing angles and investigating the possibly large corrections at the one-loop level.

The analytic results in this framework will later be applied to explicit neutrino mass models known from the literature which often introduce specific flavor symmetries in the form of discrete symmetry groups. Then, the focus will lie on producing numerical results for the mass and

mixing angle corrections in promising candidate theories, delivering data that can be compared to experiments.

WED30

16:15-16:30

Baryon Properties using Poincare Covariant Three-body Bound-state Equations

Helios Sanchis-Alepuz

Institut für Physik, Karl-Franzens Universität Graz, Graz, AUT

We discuss the calculation of the spectrum and electromagnetic properties of baryons using the combined Bethe-Salpeter/Dyson-Schwinger framework, with which one can study baryons as relativistic three-quark bound states within QCD, as recently reviewed in [1]. We present the most recent results for for Nucleon, Delta and Hyperon properties as well as the first studies of baryon excited states within this framework. We analyse the virtues and deficiencies of the widely used Rainbow-Ladder truncation and report on the status of calculations beyond that simple approximation. We finally present a program for the first-principle calculation of meson photoproduction amplitudes within this approach.

[1] G. Eichmann, H. Sanchis-Alepuz, R. Williams, R. Alkofer, C. S. Fischer, „Baryons as relativistic three-quark bound states“, to appear in Progress in Particle and Nuclear Physics.

WED31

16:30-16:45

On relativistic bound state equations

Jordi París-López

Reinhard Alkofer, Hèlios Sanchis-Alepuz

Institute of Physics, University of Graz, Graz, AUT

A fully Poincaré-covariant bound state equation derived from a Functional Renormalisation Group equation, the Wetterich equation, via

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dynamical bosonisation is critically compared to the Bethe-Salpeter-equation obtained in differently sophisticated truncations of the Dyson-Schwinger hierarchy, respectively, n -particle irreducible actions. The problem of analytically continuing to time-like momenta in both approaches is discussed. Some first preliminary results of the novel bound-state will be shown.

WED32

16:45-17:00

Performance of compressed quantum computation

Martin Hebenstreit (1)

Daniel Alsina (2), José Ignacio Latorre (2), Barbara Kraus (1)

(1) ITP, University of Innsbruck, Innsbruck, AUT (2) Universitat de Barcelona, Barcelona, ESP

It has been shown that the Ising interaction of a 1D-chain consisting out of n qubits can be simulated using a $\log(n)$ qubit universal quantum computer making use of compression of match gate circuits [B. Kraus, Phys. Rev. Lett. 107, 250503 (2011)]. Such a simulation has been performed on a five qubit nuclear magnetic resonance quantum simulator, simulating a 32 qubits chain, recently [Z. Li, H. Zhou, C. Ju, H. Chen, W. Zheng, D. Lu, X. Rong, C. Duan, X. Peng, and J. Du, Phys. Rev. Lett. 112, 220501 (2014)]. In order to test the performance of the recently available few qubit quantum computer (IBM) we perform the simulation of the compressed circuit on it and compare the results to the ones obtained using the NMR quantum computer.

WED33

17:00-17:15

Gluing methods in general relativity

Piotr Chrusciel

Faculty of Physics, University of Vienna, Vienna, AUT

Gluing methods have become by now one of the main tools to construct general relativistic initial data sets with interesting physical properties. In this talk I will review the recent progress on the topic by Carlotto

and Schoen, and by myself and Erwann Delay. I will present a new application of gluing, developed in collaboration with Lydia Bieri, to the proof that the past limit of the Trautman-Bondi mass equals the ADM mass for a large class of space-times.

OGD

JOSEF-STEFAN-HÖRSAAL

WED34

13:45-14:15

Polaron-driven (1x2) -reconstruction of rutile TiO₂ (110)

Cesare Franchini

Faculty of Physics, University of Vienna, Vienna, AUT

Surface reconstructions are structural transformations at the surface of a material that directly effect characteristics relevant to all applications involving reactivity and reaction processes. Surface reconstructions are typically due to the lack of inter-atomic forces from one crystallographic direction and the presence of broken bonds and/or polar effects at the surface. In this work we find a novel driving mechanism for surface reconstruction involving the interaction among surface polarons [1], i.e. quasiparticle originating from the coupling between excess charge carriers and the lattice phonon field. By means of a combined DFT and experimental study we explain that the reported 1x2 reconstruction of rutile TiO₂ (110), observed at high-temperature and highly reduced conditions [2, 3], is caused by the Coulomb repulsion between negatively surface polarons, which become progressively stronger with increasing oxygen vacancies (VO) concentration. At VO concentration of ~ 16.6 % the strong polaron-polaron repulsion drives the system towards an instability, which is overtaken through a structural reconstruction of the 1x2 type that increases the flexibility of the crystal and the average polaron-polaron distance. These conclusions are substantiated by the calculation of the surface energy phase

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diagram and validated by a direct comparison with STM and STS data. Our study identifies a fundamentally novel mechanism to drive surface reconstructions and resolves a long standing issue on the fundamental origin of the 1x2 reconstruction in rutile (110) [4].

Co-authors: M. Reticcioli, G. Kresse, M. Setvin, M. Schmid & U. Diebold

[1] Setvin et al., Phys. Rev. Lett. 113, 086402 (2014).

[2] Mochizuki et al., Phys. Chem. Chem. Phys. 18, 7085-7092 (2016).

[3] Wang et al., Phys. Rev. Lett. 113, 266101 (2014).

[4] M. Reticcioli et al., submitted (2016).

WED35

14:15-14:30

Charging single O₂ molecules on the TiO₂ anatase (101) surface

Martin Setvin

Michael Schmid, Ulrike Diebold

TU Wien, Vienna, AUT

The electron transfer between an O₂ molecule and a solid surface is a key mechanism in catalysis and photocatalysis. Neutral O₂ is chemically inert, while negatively charged (O₂)⁻ species readily enter chemical reactions. We use low temperature q-Plus STM/AFM to study the charging and discharging of single O₂ molecules adsorbed on the prototypical TiO₂ anatase (101) surface.

Upon adsorption, some O₂ molecules spontaneously accept electrons from the anatase substrate (n-type, 1% Nb doped). After depleting the electrons available in the near-surface region, further O₂ adsorbs as neutral species. We can use the tip to inject electrons into the neutral molecules, using a slightly positive sample bias. The electrons stay there, even though the substrate is highly conductive at all temperatures. We assume that the electron is self-trapped via the formation of a chemical bond between the (O₂)⁻ and the substrate. The bias necessary for charging the neutral molecules continuously increases with the concentration of the (O₂)⁻ species. We attribute this to the upwards band-bending induced by accumulation of negative charge at the surface. The electron can be removed from the (O₂)⁻ by the STM tip; a

bias of ~ 1.5 V is required and the molecule desorbs during the process. By illuminating the surface with UV light we show that the valence band holes can induce the same discharging mechanism as the STM tip.

WED36

14:30-14:45

Adsorption and Growth of Sexiphenyl on In₂O₃ (111)

Margareta Wagner (1)

Lynn A. Boatner (2), Michael Schmid (1), Ulrike Diebold (1)

(1) TU Wien, Vienna, AUT (2) Materials Science and Technology Division, Oak Ridge, USA

Indium oxide is one of the most important transparent conductive oxides (TCOs), and commonly used as a contact material. Sexiphenyl (6P) is a rod-like molecule and twice as long as the substrate surface lattice parameter of the (111) surface of In₂O₃ single crystals. Here, the adsorption of 6P and the monolayer structure are investigated with low temperature STM. We show that single 6P molecules have a specific adsorption site after annealing at 200°C. In empty states STM, the single 6P appears as a zig-zag line at bias voltages below +2V. At +2V the molecule starts to appear straight, which is associated with tunneling into the LUMO state. At +2.7V the apparent shape changes again into two bright features, corresponding to the LUMO+1.

No well-ordered structures are formed at sub-monolayer coverages and the molecules are spaced by a substrate lattice constant. Increasing the coverage eventually leads to a reorientation of the molecules into a densely packed monolayer structure which will be discussed in detail.

WED37

14:45-15:00

Charge transfer to organic molecules on ultrathin insulating films

Michael Hollerer (1)

Philipp Hurdax (1), Daniel Lüftner (1), Thomas Ules (1), Simon Weiß (2), Peter Puschnig (1), Mike Ramsey (1), Martin Sterrer (1)

(1) University of Graz, Graz, AUT (2) Peter Grünberg Institute, Jülich, GER

In recent years thin layers of insulators on metal surfaces have been proposed to be active in the promotion of charge transfer¹. Indeed evidence has been found for charge transfer to Au clusters on metal supported MgO (001) thin films². Here this phenomenon is investigated with scanning tunneling microscopy (STM, STS), angle resolved photoemission spectroscopy (ARPES) and DFT calculations, for the adsorption of device relevant organic molecules on MgO thin films. In this presentation we will focus on the results for pentacene (5A), where the MgO (001) is seen to both orient and immobilize the 5A. Both the STM molecular orbital images and photoemission tomography provide unambiguous evidence for charge transfer to the lowest unoccupied molecular orbital (LUMO) of 5A. The orbital tomography and the work-function measurements also allow the degree of charge transfer to be quantified. The experimental findings will be compared to DFT results and the generality of the process and its relevance to the field of organic devices will be discussed.

1 G. Pacchioni et al. (2005): Charging of Metal Atoms on Ultrathin MgO/Mo (100) Films. PRL94 (22)

2 M. Sterrer et al. (2007): Control of the Charge State of Metal Atoms on Thin MgO Films. PRL98 (9)

WED38

15:00-15:15

The initial growth of PFP on Ag (110) monitored in real-time by optical reflectance spectroscopy and photoelectron emission

Ebrahim Ghanbari

Thorsten Wagner, Andrea Navarro-Quezada, Peter Zeppenfeld

JKU, Linz, AUT

Photoelectron emission microscopy (PEEM) and optical spectroscopy are versatile tools for in-situ and real-time monitoring of physical and chemical processes occurring at surfaces [1, 2]. Recently, we have shown, how PEEM and differential reflectance spectroscopy (DRS) can be correlated to obtain an extended perspective on the electronic and optical properties of a molecular film dependent on the film thickness and morphology [3, 4]. The temporal evolution of the electron yield

in PEEM during thin film deposition cannot be explained solely by the change of the work function due to the formation of a surface dipole but it is also strongly affected by the amplitude and symmetry of the density of states at the Fermi level. In fact, dipole selection rules allow the photoelectron emission either from odd or even initial states depending on the polarization of the incident light. In this work, we have investigated the deposition of perfluoro-pentacene (PFP) on the Ag (110) surface. In particular, we applied PEEM and DRS simultaneously and synchronously during the experiment to study in detail the initial stage of growth. PEEM allows following the morphology over a 150 μm field of view whereas the spectral reflectance is averaged across a mm sized spot on the sample. In particular, the synchronous changes of the electron yield and of the optical reflectivity suggest a reorientation of the molecules on the Ag (110) surfaces during the formation of the wetting layer. Additional data from scanning tunneling microscopy and low energy electron diffraction corroborate these findings. We gratefully acknowledge the financial support by the Austrian Science Fund (FWF): No. P24528-N20.

- [1] E. Bauer, Surface Microscopy with Low Energy Electrons, Springer (2014)
- [2] R. Forker et al., Phys. Chem. Chem. Phys. 11, 2142 (2009)
- [3] E. Ghanbari et al., J. Phys. Chem. C 119, 24174 (2015)
- [4] A. Navarro-Quezada et al., Rev. Sci. Instr. 86,113108 (2015)

WED39

15:45-16:00

Monitoring the growth of organic thin films by optical spectroscopy: comparison of two differential reflectance techniques

Andrea Navarro Quezada

Ebrahim Ghanbari, Thorsten Wagner, Peter Zeppenfeld

Institute of Experimental Physics, JKU, Linz, AUT

The key for improving the performance of organic thin film devices lies in the understanding and control of their interfaces. The molecular orientation of the first monolayers on a substrate is crucial, due to the fact that it determines the structure of the subsequent layers. While

most organic molecules have a tendency to grow in an upright position on insulating and semiconducting substrates, they usually prefer a flat lying configuration on metal surfaces. Optical spectroscopy can be used to monitor physical processes occurring at surfaces and interfaces in situ and in real-time. In particular, using different polarization states of light, the orientation and conformational changes of the molecules on a surface can be determined. Due to the fact that light has a relatively large mean free path in matter, it is necessary to eliminate the optical response from the substrate in order to extract the optical properties of the surface or a thin adsorbed layer. This can be achieved by applying differential methods, namely, differential reflectance spectroscopy (DRS) or reflectance difference spectroscopy (RDS). While DRS measures the change in reflectance of a surface upon physical or chemical modification, RDS measures the change in the optical anisotropy of a surface.

In this work, we report on the in-situ monitoring of perfluoropentacene (PFP) on Ag (110) with reflectance difference spectroscopy (RDS) and polarization-dependent differential reflectance spectroscopy (pol-DRS). We compare the evolution of the surface anisotropy as a function of the coverage measured simultaneously by RDS and pol-DRS. Our results are further compared against results obtained from a combined photoelectron emission microscopy (PEEM) and pol-DRS investigation on the same system. The latter reveal a clear correlation between the average photoelectron intensity and the DRS signal obtained at 2.68 eV (a known optical transition that can be excited only with light polarized along the long axis of PFP), indicating a possible reorientation of the molecules during the initial stage of growth. In the RDS experiments we observe a change in the surface anisotropy which is consistent with the changes observed in PEEM and pol-DRS, supporting the idea of a reorganization and reorientation of the molecules during the formation of the first monolayer.

WED40

16:00-16:15

Gated Growth of Organic Rod-like Conjugated Molecules on Graphene and Hexagonal Boron Nitride Based Devices

Aleksandar Matkovic (1)

Markus Kratzer (1), Jakob Genser (1), Benjamin Kaufmann (1), Jasna Vujin (2), Borislav Vasic (2), Rados Gajic (2), Christian Teichert (1)

(1) Institute of Physics, Montanuniversität Leoben, Leoben, AUT (2) Institute of Physics, University of Belgrade, Belgrade, SRB

We focus on the hot wall epitaxial growth of sub-monolayer films of a rod-like conjugated organic semiconductor (OSC), para-hexaphenyl (C₃₆H₂₆, 6P), on the surface of graphene and hexagonal boron nitride based devices. For this purpose, mechanically exfoliated flakes supported by SiO₂/Si substrates are used and contacted in a back-gated two-point probe field effect device configuration. Charge transfer and doping of graphene channel by OSCs are investigated in situ. The effects that applied electric fields during the growth have on the resulting OSC crystallite morphologies are also presented. Furthermore, we show how residues from the lithography and annealing steps affect morphology of the grown OSC thin films. Van der Waals nature of the interface between OSCs and two-dimensional materials allows for the growth of crystallites that are several tens of micrometers large, thus minimizing the number of OSC grain boundaries within the device channel, and allowing investigations of the intrinsic properties of the OSCs.

WED41

16:15-16:30

Ultra-thin film growth of dihydrotetraazapentacene on alumina and graphene

Benjamin Kaufmann (1)

Anthony Thomas (2), Aleksandar Matkovic (1), Thomas Léoni (2), Olivier Siri (2), Rados Gajic (3), Conrad Becker (2), Christian Teichert (1)

(1) Institute of Physics, Montanuniversität Leoben, Leoben, AUT (2) CINaM, Aix Marseille Université, Marseille, FRA (3) Institute of Physics, Center for Solid State Physics and New Materials, University of Belgrade, Belgrade, SRB

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The electronic properties of azapentacenes have put them into the focus of scholarly interest due to their potential application as organic semiconductors. Here, we study ultra-thin film growth of dihydrotetraazapentacene (DHTAP) on crystalline Al_2O_3 (as a model for the gate oxide/semiconductor interface in organic field effect transistors) and exfoliated graphene (as a model system for the conductor/semiconductor interface for mechanically flexible, transparent electrodes). The added amino- and imino-groups of DHTAP lead to a dipole moment of the molecule. Compared to the well-studied organic semiconductor pentacene, it is expected that thin films of DHTAP are more stable due to dipole interaction. DHTAP is physical vapor deposited by means of molecular beam epitaxy and hot wall epitaxy. The mean thickness of the emerging films is in a range from 0.3 nm to 3 nm. Atomic force microscopy (AFM) and scanning tunneling microscopy (STM) are used to investigate the resulting growth morphologies. Both, the AFM and STM measurements showed that these morphologies strongly depend on the substrate temperatures during deposition (ranging from 220 K to 410 K). Depending on temperature, two different growth modes were found on Al_2O_3 . One leads to elongated curved, needle-like structures with a height up to about 30 nm, the other results in terraced islands which are distinctly lower. The STM results suggest for both modes that the molecules nucleate upright standing that is with their long axis nearly perpendicular to the surface plane. On graphene, the morphologies also strongly depend on temperature and show two different growth modes. In one case dendritic islands are forming and in the other case needle-like structures which tend to follow crystallographic directions of the underlying graphene substrate. These preferential orientations suggest that, in this case, the molecules nucleate with their long axis parallel to the surface plane. Compared to the curved needle-like structures found on Al_2O_3 , on graphene they are straight and exhibit a constant height of only 1 nm.

WED42

16:30-17:00

Layered Nanostructures in Proton Conductive Polymers Obtained by Initiated Chemical Vapor Deposition

Anna Maria Coclite

Paul Christian

TU Graz, Graz, AUT

Proton conductive copolymers of 1H, 1H, 2H, 2H-perfluorodecyl acrylate (PFDA) and methacrylic acid (MAA) have been synthesized by initiated Chemical Vapor Deposition (iCVD).[1] The method of copolymerization, iCVD, facilitated the tuning of the ratio between acidic -COOH groups, coming from MAA, and the hydrophobic matrix from the PFDA components.

Detailed insights into the copolymers' molecular organization were gained through an X-ray based investigation to serve as starting point for systematic studies on the relation among proton conductivity and polymer structure. Preferred crystallographic orientation (texture) in thin films frequently has a strong effect on the properties of the materials and it is important for stable surface properties. Poly-PFDA has a high tendency to give organized molecular films. Crystalline poly-PFDA have been fully obtained also by iCVD.[2] The degree of crystallinity and the preferred orientation of the perfluoro side chains, either parallel or perpendicular to the surface, can be controlled by tuning the CVD process parameters (i.e. initiator to monomer flow rate ratio, filament temperature, and substrate temperature).

The copolymers of PFDA and MAA crystallize into a bilayer structure, formed by the perfluorinated pendant chains of PFDA, perpendicular to the substrate surface. The MAA molecules form COOH enriched regions among the bilayers -parallel to the substrate surface- which can act as ionic channels for proton conduction when the acid groups are deprotonated. The interplanar distance between the bilayer lamellar structures increases by the presence of MAA units from 3.19 nm to 3.56 nm for the MAA-PFDA copolymer with 41% MAA, therefore yielding to 0.4 nm-wide channels. Proton conductivities as high as 55 mS/cm have been achieved for copolymers with 41% MAA fraction. Such ordered, layered nanostructures were never shown before for copolymers deposited from the vapor-phase and their anisotropy can be of inspiration

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for many applications beyond proton conduction. Moreover, the one-step copolymerization process has the potential to manufacture inexpensive, high quality membranes for proton exchange membrane fuel cells.

[1] C. Ranacher, R. Resel, P. Moni, B. Cermenek, V. Hacker, A. M. Coclite, *Macromolecules*, 2015, 48, 6177-6185

[2] A. M. Coclite, Y. J. Shi, K. K. Gleason, *Adv. Funct. Mater.* 2012, 22, 2167-2176

WED43

17:00-17:15

Measurements of viscoelasticity and adhesion force of polymer materials with large radius AFM tips

Christian Ganser (1)

Caterina Czibula (1), Jakob Manhart (2), Simone Radl (2), Sandra Schlögl (2), Ulrich Hirn (3), Christian Teichert (1)

(1) Montanuniversitaet Leoben, Institute of Physics, Leoben, AUT (2) Polymer Competence Center Leoben GmbH, Leoben, AUT (3) Graz University of Technology, Christian Doppler Laboratory for Fiber Swelling and Paper Performance, Graz, AUT

The investigation of cellulose and artificial polymer surfaces with atomic force microscopy (AFM) allows to access properties of these materials, such as hardness and elastic modulus [1], but also viscosity and adhesion forces on the nanometer scale. Here, the cellulosic surfaces are pulp fibers. The knowledge of viscoelastic properties of pulp fibers is interesting for the refining process, where fibers are loaded at high speeds. Additionally, the viscoelasticity will naturally influence the formation of a bond between two fibers.

The functional polymer is a hydrogenated carboxylated nitrile butadiene rubber with photo-sensitive anthracene pendant groups, which can be reversibly cross-linked and de-linked by illuminating it with UV light [2]. In this case, the adhesion force is the most interesting quantity: by simply illuminating the polymer with UV light it is possible to control the "stickiness" of the surface. However, due to the viscoelastic nature of this polymer, the measured adhesion force will also change over time. The reason is that the contact area between tip and sample will

increase and so will the adhesion force.

Such information is only meaningful when the sample surface is smooth compared to the tip size. Usually, the sample surface cannot be influenced, e.g., pulp fibers have a fixed roughness. Therefore, we employed AFM tips with a large radius so that the sample surfaces would be smooth in comparison. Using this method, it was possible to measure viscoelastic properties of pulp fibers and time dependent adhesion forces on stimuli responsive polymer surfaces.

[1] Ganser C., Kreiml P., Morak R., Weber F., Paris O., Schennach R., Teichert C. *Cellulose*, 22 (2015), 2777-2786

[2] Radl S., Kreimer M., Griesser T., Oesterreicher A., Moser A., Kern W., Schlögl S. *Polymer*, 80 (2015), 76-87

PHYD

ERWIN-SCHRÖDINGER-HÖRSAAL

WED44

13:45-14:15

Activities of the ICTP in Physics for Development

Joseph Niemela

ICTP, Trieste, ITA

The Abdus Salam International Centre for Theoretical Physics (ICTP) is an international research institute for physical and mathematical sciences, founded in 1964 in Trieste, Italy by Pakistani Nobel Laureate Abdus Salam. Its primary mission is to foster the growth of advanced studies and research in physical and mathematical sciences, with a special emphasis on developing countries. The talk will cover some of the programs developed for this purpose, in addition to bottom-up programs addressing the need for science education and entrepreneurship, in collaboration with other partners.

To date, over 130,000 scientists from 188 different countries have

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visited the center for scientific exchange and training in addition to those reached by ICTP activities outside of Trieste.

WED45

14:15-14:45**Physics for Sustainable Development**Barbara Capone*Faculty of Physics, University of Vienna, Vienna, AUT*

Sustainable development is one of the most ambitious goals of modern society. International politics is aiming at the design and realisation of sustainable cities, and latest technological developments are, day after day, heading in such a direction.

Nevertheless, while on the one side modern cities are being designed, projected and realised, a huge part of the world wide population lives in emergency situations, e.g. without access to energy or water sanitation. In such a framework, the implementation of existing technologies and the design of novel materials in the direction of renewable energies, water sanitation and energy storage is an ambitious goal that, as scientists and in particular as material physicists, we felt the urge of pursuing.

In this talk we will present the work of Sunshine4Palestine (S4P), an NGO funded by a group of physicists and engineers whose aim is finding solution to water and energy emergency situation. S4P is active of the realisation of a photovoltaic plant on a hospital in Gaza, Palestine. Previously to the intervention of the NGO, the hospital could only operate 4 hours a day, due to the energy shortages that are affecting the strip. After the installation of the S4P designed PV plant, the structure is operating 17 hours a day, with an increase of about 175% of the total patients treated, with peaks of 500% in sectors as the obstetric department.

Parallel to the implementation projects, that are currently seeing the photovoltaic conversion of the water distribution system - for both domestic and agricultural purposes - in rural areas in Gaza that are only receiving water for a few hours per week due to energy shortages, the NGO is developing different research lines. As part of an international consortium made of 10 universities and industrial partners - S4P

is aiming at designing novel nanomaterials for a sustainable water sanitation. Moreover the NGO is dedicating a big effort in an outreach activity by both building up a know-how transfer in every intervention areas by forming local teams of technicians, and by carrying on a both an academic scientific exchange and a divulgation project that is involving universities and schools both in the West Bank and in Gaza.

WED46

14:45-15:00

Science4People - Scientific Popularization for young people in the Gaza Strip

Chiara Cardelli

Faculty of Physics, University of Vienna, Vienna, AUT

Modern society is characterized by important scientific achievements, leading to technological progresses that are improving the everyday quality of life. However, this development affects especially the richest areas of the world, while million of human beings are facing humanitarian crisis leading to a poor quality of life. In such a context the potential of a scientific and technological know-how transfer to populations with poor living conditions is striking. Sunshine4Palestine is a technical NGO, founded by a group of physicists and engineers, focusing on different projects aimed at improving the everyday living conditions in areas of the world where access to basic services, as a continuous energy distribution or water sanitation, is prohibitive. In such a context, the outcomes of a scientific development might become the key for an innovative and life changing path for the local population, bridging the gap between the existing difficulties and possible solutions. Hence scientific popularization can play a central role to fill the gap between scientists and final users, teaching a common language to the two communities to speak of problems and simple solutions, in order to make scientific knowledge a central component of culture and of social awareness. As scientific team of Sunshine4Palestine we are organizing, in partnership with students of the Applied Science College of the Al-Aqsa University in Gaza and in West Bank, a scientific popularization project for young scholars in the Gaza Strip. The project aims at performing experiments focusing on the topics of water and renewable energies.

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The experiments have a double aim: on one side they will teach the children how to deal with problems by encouraging critical and proactive thinking, on the other side they will put their mind in a positive and confident state regarding their everyday problems. The final aim of the project is to start the first science popularization program in the Gaza Strip, that will be undertaken and carried on by the local University students. Moreover part of this project, includes a scientific exchange between European Scientists and their colleagues of the Palestinian University, though seminars on the research topics carried out from the Sunshine4Palestine scientific team. This stage aims at encouraging possible future scientific collaborations between European and Palestinian scientists. The project will be carried out in collaboration with the Young Mind initiative of the European Physical Society and with Scientists for Palestine, an international network of scientist who will organize an advanced physics school in the West Bank.

PIE

ERWIN-SCHRÖDINGER-HÖRSAAL

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15:45-16:00

Selbstständigkeit im Bereich F&E in der Dünnschichttechnologie

Georg Strauss

Universität Innsbruck, Innsbruck, AUT

Der Weg, heraus einer relativ geschützten Forschungsumgebung an der Universität, hinein in die Selbstständigkeit im industriellen Umfeld scheint kein leichter zu sein, ist aber dennoch gerade für PhysikerInnen eine echte Alternative. Das Physikstudium bietet hervorragende Voraussetzungen hinsichtlich der naturwissenschaftlichen und technologischen Ausbildung und animiert zum selbstbestimmenden und eigenständigen Arbeiten und Entscheiden. Die echten Herausforderungen liegen am Weg in die Selbstständigkeit und der Unternehmensgründung im Bereich der wirtschaftlichen Umsetzung der innovativen Ideen

und marktstrategischen Ausrichtung des Unternehmens, um eine nachhaltige Struktur aufzubauen.

Dr. Georg Strauss hat Physik an der Universität Innsbruck studiert, dort mehrere Jahre als wissenschaftlicher Assistent gearbeitet und hat sich 2003 im Umfeld der Oberflächen- und Dünnschichttechnologie mit dem Unternehmen PhysTech Coating Technology selbstständig gemacht.

Aus diesen Erfahrungen der Unternehmensgründung, von der Start-Up Phase bis hin zu einem etablierten Technologieunternehmen, wird Dr. Georg Strauss berichten und die Hürden, Notwendigkeiten, Erfolge und Chancen aufzeigen und diskutieren und kann dabei einen Einblick in eine interessante Berufswelt geben.

WED48

16:00-16:15

Als Physiker zwischen Kristallen und Kraftwerken

Peter Korczak

ehem. Siemens AG, Salzburg, AUT

Es wird berichtet über einen wechselvollen Berufsweg als Physiker in der Industrie, zwischen Forschung, neuen Technologien und technischem Management. Nach Arbeiten über Silikat-Kristallstrukturen an der TU Wien, ein Sprung in die Reaktorphysik als Mitarbeiter der Planungsgesellschaft für das KKW Zwentendorf. Infolge Projektverzögerungen, Rückkehr in die industrielle Forschung, im AEG Forschungsinstitut Frankfurt a. M. Dort Herstellung von Einkristallen für optische Datenspeicher und Gasanalysegeräte. Nach Berufung zum Vorstandsassistenten für Forschung im AEG Konzern, Rückkehr nach Wien, über die AEG Anlagentechnik, zur Siemens AG in die Kraftwerksplanung. Avancement vom Vertriebsleiter zum Bereichsleiter und Direktor für Energieerzeugung, umfassend Wasser-, Gas- und Dampfkraftwerke. Parallel dazu Aufbau des neuen Arbeitsgebietes Photovoltaik und Realisierung der Pilotprojekte in Österreich. Abschließend Ruf nach Salzburg als Siemens-Direktor mit 350 Mitarbeitern für alle Arbeitsgebiete des Konzerns. In Salzburg Gründung eines Kompetenzzentrums für Kleinwasserkraftwerke und erstmaliger Einsatz von CIS-Solarmodulen aus Dünnschicht-Produktion, als letzter Photovoltaik - Meilenstein.

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WED49**16:15-16:30****Funding Research and Development - Austria and Europe**Olaf N. Hartmann*Austrian Research Promotion Agency, Vienna, AUT*

Subsequent to my physics studies in Gießen and Darmstadt (Germany), concluded with the PhD in 2003, I spent several years in research in experimental hadron and nuclear physics, before joining the Austrian Research Promotion Agency FFG in 2012. FFG is the Austrian funding agency for industrial R&D, being the operational body for many national funding programmes, expert organization, national contact point for the European framework programmes etc. I am working in the programme management of the joint European SME funding programme Eurostars and as internal reviewer.

In the talk I will present an overview of the activities of the FFG and possible profiles for scientists in the various fields of activities.

WED50**16:30-16:45****Biophysik: die Brücke zwischen Biologie und Physik**Eva Sevcsik*TU Wien, Vienna, AUT*

Die moderne Biophysik ist eine stark interdisziplinäre Wissenschaftsrichtung, die die Methoden und Zugänge der Physik anwendet, um biologische Systeme zu beschreiben. In der wissenschaftlichen Forschung arbeiten Physiker, Biologen, Chemiker und Materialwissenschaftler gemeinsam im selben Labor und bringen ihre jeweilige Expertise ein. Frau DI Dr. Sevcsik forscht als Universitätsassistentin in einem Biophysiklabor an der TU Wien. In diesem Vortrag gibt sie einen Einblick in Karrierewege in der universitären Forschung im Bereich der Biophysik, den Forschungsalltag, und das spannende Gebiet der Membranbiophysik.

WED51

16:45-17:00

Strengths and opportunities of a physicist in the non-academic sector

Rafael Reiter

Vienna, AUT

The road to a physics degree is long, winding and dry, and a lot of students, including myself not too long ago, ask themselves what possibly lies ahead in the non-academic sector. The methods acquired in theoretical and experimental physics may seem far from industrial application, but in my experience, a physicist brings optimization skills to the table that are needed quite early in a growing, mixed team of engineers. I've been working for two hi-tech lithography companies where I was initially hired as a software engineer, but also worked on optimization problems, physical modelling and product development, resulting in four patents so far.

AMP

SMI SEMINARRAUM

WED52

13:45-14:00

Transient XUV absorption spectroscopy of laser dressed krypton with attosecond resolution

Enikoe Seres (1)

Jozsef Seres (1), Carles Serrat (2), Shinichi Namba (3)

(1) TU Wien, Vienna, AUT (2) Universitat Politècnica de Catalunya, Terrassa, ESP (3) Hiroshima University, Hiroshima, JPN

Transient absorption spectroscopy has an old tradition. Since the early 60's the scientific community refers to "x-ray dressed atoms" and since the early 90's to "laser dressed atoms" [1,2]. In the later case, an atom

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is illuminated with a laser field strong enough to modify, by its electric field, the unoccupied levels of the atom. A weak XUV field is used as probe to measure how the levels changed by means of time-resolved x-ray absorption spectroscopy [3]. The rapidly exploding, authentic techniques of attosecond physics confer transient absorption spectroscopy an enormous importance due to the strong binding to chemical physics and chemistry. Our aim was to measure the time-resolved XUV absorption of neutral Kr gas at around 90 eV. Krypton was earlier measured in its ionized states [4]. It has absorption between 90 and 95 eV [5] containing transitions between the 3d inner-shell and the unoccupied np levels. The two unoccupied levels of 5p and 6p differ by 1.4 eV, making Kr very suitable for resonantly coupling the two levels with the broad spectrum of a femtosecond Ti:sapphire laser at 1.5 eV and making the dressing phenomenon even stronger. We examined the fast absorption changes from the 3d core level caused by the laser field. For the experiment, we used the 30 fs pulses of a Ti:sapphire laser systems which was focused with a concentric mirror-pair. The outer mirror focused a part of the laser beam to the Kr gas and served as a dressing beam to merge with 5p and 6p levels. The small mirror focused the laser beam to a Ne filled gas jet to generate high harmonics for probe. This central mirror was movable providing a temporal resolution of 0.2 fs. The transmitted XUV probe beam was measured with a McPherson x-ray spectrometer. Our experimental results show a fast and a slow oscillation at the 3d to 5p transition (91.2 eV). The fast is driven by the electric field of the dressing laser, and the slow change is the consequence of the multiphoton excitation of the Kr atoms by the laser pulse. We observed also beat oscillation with ~10 fs interval, which can be the effect of the coupling between the 5p-6p and 6p-7p dressed levels. This work was supported by the EC's 7th Framework Program (grant 284464, Laserlab Europe HIJ-FSU0019152 and HIJ-FSU001975); the ERC Starting Grant 258603 and the EU-FET-Open 664732 „nuClock“; the Spanish Ministry of Economy and Competitiveness through “Plan Nacional” (FIS2014-51997-R); the Japanese Society for the Promotion of Science “KAKENHI 22340174”.

[1] K. Codling, P. Madden, Phys. Rev. Lett. 12, 106-108 (1964)

[2] K.-J. Boller, et al., Phys. Rev. Lett. 66, 2593 (1991)

[3] E. Seres, J. Seres, C. Spielmann, Appl.Phys A 96, 43-50 (2009)

[4] E.Goulielmakis, et al., Nature 466,739-744 (2010)

[5] G. C. King, et al., J. Phys. B 10, 2479-2495 (1977)

WED53

14:00-14:15

Probing the formation of PAH interstellar dust grains

Marcelo Goulart (1)

Thomas Kurzthaler (1), Bilal Rasul (2), Lorenz Kranabetter (1), Martin Kuhn (1), Alexander Kaiser (1), Albrecht Lindinger (3), Andrew Ellis (4), Paul Scheier (1)

(1) University Innsbruck, Innsbruck, AUT (2) University of Sargodha, Sargodha, PAK (3) Freie Universität Berlin, Berlin, GER (4) University of Leicester, Leicester, GBR

Polycyclic aromatic hydrocarbons (PAH) are abundant molecules in the universe, more precisely in interstellar clouds, and are associated with infrared emission lines commonly observed [1]. In these clouds PAH molecules can undergo aggregation and form soot-like particles or dust grains. The abundance of many chemical species in the interstellar medium, remarkably H₂, can be explained by reaction pathways that take place on the surface of dust grains [2].

The use of a cryogenic matrix, notably superfluid helium nanodroplets (HND), is an important experimental technique mainly due to its uncommon behavior at extremely low temperatures (0.4 K) and its ability to capture virtually almost any atom or molecule that collides with it [3], making it a perfect laboratory for simulating the conditions where the PAH aggregation and reactions take place. Herein we report a new mass spectrometric technique on the investigation of PAH aggregates formation. By growing PAH clusters inside HND and subsequent doping them with atomic or molecular species it is possible to acquire conformational information by analyzing the first solvation shell behavior. Intensity anomalies on the mass spectra related to the stability of the molecular complexes, known as magic numbers, are used to identify the most likely aggregation patterns of PAH dust grains.

Acknowledgement: this work was supported by the Austrian Science Fund FWF, I978, P26635, M 1908-N36.

1.Tielens, A.G.G.M., et al. Astrochemistry: From molecular clouds to planetary systems. in Symposium of the International Astronomical Union. 2000. Sogwipo, Cheju, Korea: Astronomical Society of the Pacific (January 2000).

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2.Hollenbach.D and E.E. Salpeter, Surface recombination of hydrogen molecules. *Astrophysical Journal*, 1971. 163 (1): p. 155-164.

3.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.

WED54

14:15-14:30

Photo-induced dynamics in selenophene molecules probed by femtosecond transient XUV absorption spectroscopy

Florian Lackner (1,2)

Adam S. Chatterley (2), Chaitanya D. Pemmaraju (2), Kristina D. Closser (2), David Prendergast (2), Daniel M. Neumark (1,2), Stephen R. Leone (1,2), Oliver Gessner (2)

(1) UC Berkeley, Berkeley, CA, USA (2) Lawrence Berkeley National Laboratory, Berkeley, CA, USA

We report on the ring-opening and dissociation dynamics of strong-field ionized selenophene (C_4H_4Se), studied by transient XUV absorption spectroscopy at the Se 3d edge. The table-top experiments are facilitated by high-order harmonic generation coupled with a gas phase transient XUV absorption setup that is optimized for the study of organic compounds. Employing element-specific core-to-valence transitions, the ultrafast molecular dynamics are monitored from the perspective of the well-localized Se atoms. Spectral features are assigned based on first principles TDDFT calculations for a large manifold of electronic states. The experiments reveal, in particular, insight into the strong-field induced ring-opening dynamics in the selenophene cation, which are traced by the emergence of non-cyclic molecules as well as the liberation of Se^+ ions within an overall time scale of approximately 170 fs. The temporal behavior of both features can be modeled within a sequential two-step model employing two identical time scales $\tau_1 \approx \tau_2 \approx 80$ fs. We thus propose that both products may be associated with dynamics on the same electronic surfaces but with different degrees of vibrational excitation. The combined experimental and theoretical results suggest a close relationship between σ^* excited cation states and the observed ring-opening reactions. The findings demonstrate that the combination of femtosecond time-resolved core-level spectroscopy with ab initio

estimates of spectroscopic signatures provide new insights into complex, ultrafast photochemical reactions such as ring-opening dynamics in organic molecules in real-time and with simultaneous sensitivity for electronic and structural rearrangements.

WED55

14:30-14:45

Parametric amplification and phase matching in high harmonic generation

Jozsef Seres (1)

Carles Serrat (2), David Roca (2), Josep M. Budesca (2), Enikoe Seres (1), Bastian Aurand (3), Andreas Hoffmann (4), Shinichi Namba (5), Thomas Kuehl (6), Christian Spielmann (4)

(1) TU Wien, Vienna, AUT (2) Universitat Politècnica de Catalunya, Terrassa, ESP (3) Universität Düsseldorf, Düsseldorf, GER (4) Friedrich Schiller University, Jena, GER (5) Hiroshima University, Hiroshima, JPN (6) GSI Helmholtz Centre for Heavy Ion Research, Darmstadt, GER

High-order parametric interactions to produce coherent ultrashort pulses in the extreme ultraviolet within the framework of high-order harmonic generation (HHG) are attracting attention nowadays. Beyond the first experimental demonstration [1], both perturbative [2] and non-perturbative [3,4] theoretical descriptions were developed based on classical [5] and quantum mechanical [2,6] considerations. The observed exponential and hyperbolic increase of the generated short wavelength radiation via the medium length or the medium density rose debate on the rule of the phase matching in the process.

Our numerical simulations are based on the quantum-mechanical description of HHG using the strong field approximation [2], which is extended by considering propagation and phase matching effects [6]. High-order parametric amplification was studied in a gas medium driven by a strong near-infrared (NIR) laser field both unseeded or self-seeded and externally seeded configurations.

We demonstrate that the strong-field theory in the frame of high harmonic generation fully supports the appearance of both the avalanche-like and saturation effects in the amplification of extreme ultraviolet attosecond pulse trains. Experimental studies and subsequent model calculations were performed on He gas driven by intense

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30-fs-long laser pulses from a Ti:sapphire laser system, which was seeded with an attosecond pulse train at 110 eV generated in a separated Ne gas jet. We theoretically separated and identified different physical processes taking part in the interaction and demonstrated [6] that X-ray parametric amplification [1] dominates over others. Furthermore, the observed propagation and saturation are in contradiction to regular phase matching and exclude pressure induced phase matching as a possible explanation. It can be explained correctly only by considering parametric amplification of the XUV pulse train. These theoretical predictions are fully supported by experiment results [6,7]. We work further to extend our model to higher photon energies. This work was supported by the Spanish Ministry of Economy and Competitiveness through “Plan Nacional” (FIS2014-51997-R); German DFG grant TR18; the Japanese “Research Foundation for Opto-Science and Technology”; EC’s 7th Framework Program (grant 284464, Laserlab Europe HJ-FSU0019152 and HJ-FSU001975); ERC project 664732- nuClock.

- [1] J. Seres, et al., Nat. Phys. 6, 455-461 (2010)
- [2] C. Serrat, Phys. Rev. Lett. 111, 133902 (2013)
- [3] L.V. Dao, et al., Nat. Comm. 6, 7175 (2015)
- [4] V. V. Strelkov, Phys. Rev. A 93, 053812 (2016)
- [5] J. Seres, et al., Phys. Rev. A 86, 013822 (2012)
- [6] C. Serrat, et al., Opt. Express 24, 8028-8044 (2016)
- [7] J. Seres, et al., Sci. Rep. 4, 4254 (2014)

WED56

14:45-15:00

Non-planar femtosecond enhancement cavity-based VUV frequency comb

Georg Winkler

Jakob Fellinger, Jozsef Seres, Enikoe Seres, Thorsten Schumm

TU Wien, Vienna, AUT

External passive femtosecond enhancement cavities (fs-ECs) are an attractive tool to increase the efficiency of non-linear conversion processes like high harmonic generation (HHG) at high repetition rates [1], and are crucial in the realization of short-wavelength frequency combs

for high-precision spectroscopy applications in particular. We introduce a novel three-dimensionally folded variant [2] of the typical planar bow-tie resonator geometry that guarantees circular beam profiles, maintains linear polarization, and allows for a significantly tighter focus as well as a larger beam cross-section on the cavity mirrors. Starting with a low-power Ti:Sapphire VUV frequency comb centered at 800 nm, we used the novel EC design to generate the 5th harmonic at 160 nm, specifically targeting spectroscopy of the low-energy isomer state of Thorium-229 [3,4]. The scheme could be equally beneficial for use cases involving much higher pump powers, where the damage threshold of the cavity mirrors becomes a major concern.

The seed oscillator used in the setup generates 25-fs-long pulses with 900 mW of average power at a repetition rate of 108 MHz (FC8004, Menlo Systems). To obtain the transform-limited short pulse inside the cavity, the cumulative group delay dispersion (GDD) added by mode-matching optics, vacuum chamber window, incoupling mirror substrate and propagation in air was pre-compensated by multiple bounces on chirped mirror pairs. The three-dimensional arrangement of the 6 planar folding mirrors and 2 focusing mirrors (focal length of 75 mm) in the EC, allows producing peak laser intensity beyond 10^{13} W/cm², as required for HHG in xenon gas. The generated harmonics (including the fifth harmonic at the target wavelength of 160 nm) were coupled out with 100- μ m-thick BK7 glass plate and measured with a (McPherson Model 234) VUV spectrometer. Using the new design, an intracavity pulse duration of about 30 fs and an overall enhancement factor of 250 was obtained. We also demonstrated tunability of the beam waist in the intracavity focus between 10 μ m and 22 μ m while preserving the high enhancement factor of the cavity.

This work was supported by the FWF Project Y481, the ERC Starting Grant 258603 and the EU-FET-Open 664732 „nuClock“.

[1] C. Gohle, et al., Nature 436, 234-237 (2005)

[2] G. Winkler, et al., Opt. Express 24, 5253-5262 (2016)

[3] B. Beck, et al., Phys. Rev. Lett. 98, 142501 (2007)

[4] P. Dessoic, et al., J. Phys.: Condens. Matter 26, 105402 (2014)

WED57

15:00-15:15**Interpolation of Potential Energy Surfaces Using Force Field Methods**Ralf Meyer

Andreas W. Hauser

Institut für Experimentalphysik, TU Graz, Graz, AUT

Highly accurate interpolation techniques for potential energy surfaces bear the potential to speed up quantum chemistry calculations by reducing the number of necessary ab initio evaluations. The most common interpolation methods, such as high dimensional cubic splines, interpolating moving least squares (IMLS), [1] or neural network approaches, [2] are motivated strictly by mathematical arguments and require a large number of ab initio points.

In this work we present a combination of the interpolating moving least squares formalism with physically motivated potential energy expansions of common force fields. Since these force fields can already provide reasonable predictions for the functional course of the potential energy surface, an interpolation to the same accuracy can be done using less reference points than needed by common surface fitting methods. In a first test, we analyze the performance of our method by a direct comparison to the time propagation of free gas molecules at a given temperature, evaluated with density functional theory and Born-Oppenheimer molecular dynamics.

[1] G. G. Maisuradze, D. L. Thompson, J. Phys. Chem. A 2003, 107, 7118-7124

[2] S. Manzhos, X. Wang, R. Dawes, T. Carrington Jr., J. Phys. Chem. A 2006, 110, 5295-5304

WED58

15:45-16:00

Interference Fringes Controlled with Non-Interfering Photons

Armin Hochrainer

Radek Lapkiewicz, Mayukh Lahiri, Gabriela Barreto Lemos, Anton Zeilinger

IQOQI Vienna, Vienna, AUT

If two separate sources produce photon pairs (signal and idler) by spontaneous parametric down conversion (SPDC), the two resulting signal beams are in general mutually incoherent. However, lowest-order interference between the signal beams can be observed, if no information is accessible, which source generated a particular photon pair. This can be achieved by aligning the idler beams from the two sources such that they are indistinguishable. This phenomenon was termed induced coherence without induced emission [1,2] and was recently applied for imaging [3]. In such an experimental situation, path-distinguishability can be introduced by attenuating the idler beam from one source. It has been shown that if this attenuation is implemented by a partially transmissive filter, the resulting visibility is proportional to the transmission coefficient [1,2]. We analyze, how the interference of the signal beams is affected, if path distinguishability is introduced different way, by misaligning the two idler beams. We show that this leads to the observation of spatial interference fringes due to the momentum correlation of photons generated in SPDC. The interference pattern depends on the alignment of the idler beam in an analogous way as the fringes created in a traditional division-of-amplitude interferometer depend on the relative alignment of the two interfering beams. We demonstrate that in contrast to fringes generated by division-of-amplitude, the pattern is characterized by an effective wavelength, which corresponds to a combination of the wavelengths of the involved physical beams. Moreover, we show how the visibility of the pattern depends on the momentum correlation between signal and idler photons.

[1] X. Y. Zou, L. J. Wang, and L. Mandel, „Induced coherence and indistinguishability in optical interference,“ *Phys. Rev. Lett.* 67, 318 (1991).

[2] L. J. Wang, X. Y. Zou, and L. Mandel, „Induced coherence without induced emission,“ *Phys. Rev. A* 44, 4614 (1991).

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[3] G. B. Lemos, V. Borish, G. D. Cole, S. Ramelow, R. Lapkiewicz, and A. Zeilinger, „Quantum imaging with undetected photons,“ *Nature* 512, 409–412 (2014).

WED59

16:00-16:15

Experimental Verification of a Causally Non-Separable Process

Giulia Rubino

Faculty of Physics, University of Vienna, Vienna, AUT

Investigating the role of causal order in quantum mechanics has recently revealed that the temporal distribution of events may not be a-priori well-defined in quantum theory. While this has triggered a growing interest on the theoretical side, the existence of processes without a causal order is an experimental question. Although a previous experiment has shown indirect evidence for causally non-ordered effects by showing a predicted computational enhancement, a concrete verification of causal non-separability has not yet been achieved. To that end, here we report the first decisive demonstration of a causally non-separable process. To do so, we make use of a recent theoretical result to quantify the causal non-separability of a given process by measuring a ‚causal witness‘. A causal witness is designed to yield a negative value only if the process under examination is not consistent with any possible process with a well-defined causal order. We measured a causal witness for a process built in our laboratory, and our results demonstrate by more than 6 standard deviations, that we have experimentally implemented a process which does not have definite causal order. - SFB-FOQUS submission

WED60

16:15-16:30

Experimental test of Hyper-Complex Quantum Theories

Lorenzo Procopio

Lee Rozema

Faculty of Physics, University of Vienna, Vienna, AUT

One of the most successful theories in physics until now is quantum mechanics. However, the physical origins of its mathematical structure are still under debate, and a “generalized” quantum theory to unify quantum mechanics and gravity is still missing. Recently, in an effort to better understand the mathematical structure of quantum mechanics, theories containing the essence of quantum mechanics, while also having a broader description of physical phenomena, have been proposed. These so-called “post-quantum theories” have only been recently tested at the lab. In this talk, I will present the results of our experimental test using single photons to probe one of these post-quantum theories; namely, hyper-complex quantum theories. Interestingly, in hyper-complex theories simple phases do not necessarily commute. To study this effect, we apply two physically different optical phases, one with a positive and one with a negative refractive index, to single photons inside of a Sagnac interferometer. Through our measurements we are able put bounds on this particular prediction of hyper-complex quantum theories.

WED61

16:30-16:45

Experimental study of spin-orbit coupled Bose gas

Sicong Ji

Atominstytut, TU Wien, Vienna, AUT

Spin-Orbit Coupling is a phenomenon describes the relation between particles’ velocity and quantized spin. It leads to numerous phenomena in electron systems, such as topological insulator, quantum Hall effect and Majorana fermions. Artificial SO coupling in ultracold neutral atoms provides the opportunity to study such phenomena in bosonic systems, which exhibit superfluidity and various symmetrybreaking condensate phases. In general, a richer structure of symmetry breaking results in a nontrivial finite-temperature phase diagram, but the thermodynamics of the SO-coupled Bose gas at finite temperature remains unknown both in theory and experiment. In the first part, we experimentally determine a new finite-temperature phase transition that is consistent with the transition between the stripe ordered phase and the magnetized phase. We also observe that the magnetic phase and

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the Bose condensate transitions occur simultaneously as temperature decreases. We determine the entire finite-temperature phase diagram of the SO-coupled Bose gas, thus illustrating the power of quantum simulation.

In the Second part, we find the SO coupling can also lead to a non-trivial excitation spectrum. Using Bragg spectroscopy, we study the SO coupled Bose-Einstein Condensate of 87 Rb and find the roton-maxon structure in the lowest branch of the excitation spectrum. We also notice, with the Raman coupling strength decreasing, a roton-mode softening will happen, as a precursor of phase transition to super solid that spontaneously breaks spatial translational symmetry. Furthermore, we also determine a phonon-mode softening as the geometry phase transition point of the excitation spectrum by measuring the sound velocities. This work provides a new way to simulate and study the system with long-range system.

WED62

16:45-17:00

Demonstration of measurement-only blind quantum computing

Marie-Christine Röhsner (1)

Chiara Greganti (1), Stefanie Barz (1), Tomoyuki Morimae (2), Philip Walther (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Gunma University, Kiryu-shi Gunma-ken, JPN

Blind quantum computing allows for secure cloud networks of quasi-classical clients and a fully-fledged quantum server. Recently, a new protocol has been proposed, which requires a client to perform only measurements. We demonstrate a proof-of-principle implementation of this measurement-only blind quantum computing, exploiting a photonic setup to generate four-qubit cluster states for computation and verification. Feasible technological requirements for the client and the device-independent blindness make this scheme very applicable for future secure quantum networks.

WED63

17:00-17:15

Coherent deflectometry in a matter-wave interferometer for biomolecules

Lukas Mairhofer

Faculty of Physics, University of Vienna, Vienna, AUT

Matter-wave interference has been demonstrated for molecules with up to 10.000 amu (Eibenberger, PCCP 15, 2013). The sensitivity of matter-wave interferometers to external forces enables interference enhanced deflectometry with high spatial resolution. The interference pattern itself provides a ruler that is sensitive to shifts of a few nanometers. If a deflecting field maintains the spatial coherence of the molecule's center-of-mass wave-function, the interferometer thus can enhance the resolution of deflection measurements by four orders of magnitude compared to classic ballistic deflectometry. Such experiments were conducted with static electric fields (Eibenberger, NJP 13, 2011). Also the absorption of single photons suffices to shift the interference pattern (Eibenberger, PRL 112, 2014). This allows us to determine of the magnetic, electric and optical properties of neutral molecules in the gas phase. The investigation of biomolecules is of special interest as they have a rich bond-structure that influences their behaviour. The project builds on an existing matter-wave interferometry setup with the aim of extending it to an instrument for high precision measurements of these properties. We will report on the first successful quantum interference of a range of biomolecules such as polypeptides and vitamins.

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VICTOR FRANZ HESS PRIZE WINNER TALK

LISE-MEITNER-HÖRSAAL

THU01

11:00-11:30

How General Is Holography?

Max Riegler (1)

Daniel Grumiller (1), Arjun Bagchi (2), Rudranil Basu (3)

(1) Institut für theoretische Physik, TU Wien, Vienna, AUT (2) Massachusetts Institute of Technology, USA (3) Saha Institute of Nuclear Physics, IND

The holographic principle is a proposed duality between a theory of (quantum) gravity in $D+1$ dimensions and a quantum field theory in D dimensions that is located at the boundary of the gravity theory. Since most explicit realizations of such a holographic correspondence either involve string theory and/or spacetimes with constant negative curvature a natural question to ask is: „How General Is Holography?“. In this talk I will give an overview of current research directions that provide ways of better understanding the generality of the holographic principle. I will focus on $2+1$ dimensions where many aspects of the holographic principle can be checked explicitly. I will present a way of establishing new holographic correspondences in this setup as well as a brief introduction to higher-spin symmetries. After this I will focus on a new holographic correspondence involving asymptotically flat spacetimes where I will present an explicit, nontrivial check of this correspondence by computing holographic entanglement entropy.

MAX AUWÄRTER PRIZE WINNER TALK

LISE-MEITNER-HÖRSAAL

THU02

11:30-12:00

Diffusion, rotation and friction: studying the dynamics of a molecule on a surface

Barbara A. J. Lechner (1,2)

Holly Hedgeland (2), Andrew P. Jardine (2), William Allison (2), B. J. Hinch (3), John Ellis (2)

(1) Chemistry Department, Technische Universität München, Garching, GER, (2) Cavendish Laboratory, University of Cambridge, Cambridge, GBR, (3) Department of Chemistry and Chemical Biology, Rutgers University, NJ, USA

The efficiency of a solid catalyst, the formation of self-assembled molecular networks, and the growth of thin film coatings – processes occurring on the surfaces of solids are governed by the dynamic properties of adsorbate species and by their interaction with each other. A fundamental understanding of the forces guiding surface diffusion and growth processes is thus of utmost importance for many branches of the chemical industry. In the present talk I will illustrate how the experimental observation of the dynamics of molecules adsorbed on well-defined surfaces extends our molecular level understanding of inter-adsorbate and adsorbate–surface interactions in complex surface dynamical systems.

Helium spin echo (HeSE) spectroscopy is uniquely suited to investigate the diffusion and vibrational motion of relatively small, molecular adsorbates as it probes surface dynamics on pico- to nanosecond time scales. Comparing a range of aromatic adsorbates shows that the diffusion is largely independent of adsorbate–substrate interaction strength. On Cu (111), cyclopentadienyl (C₅H₅) forms an ionic bond, pyrrole (C₄H₄NH) is physisorbed and thiophene (C₄H₄S) chemically bonded, yet all three adsorbates move in single jumps between preferred adsorption sites over low activation barriers of 40–60 meV [1-3]. In addition, thiophene exhibits rotational motion around the S-Cu anchor point and a flapping perpendicular to the substrate. HeSE measurements

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further give a handle on the single-molecule friction of these mobile adsorbates, which was found to be surprisingly high compared to atomic adsorbates of comparable mass. Moving to more asymmetric molecules, we found that pentacene molecules move along rails parallel and perpendicular to a well-ordered pentacene monolayer and can rotate to switch between diffusion directions [4].

[1] H. Hedgeland, B.A.J. Lechner, F.E. Tuddenham, A.P. Jardine, W. Allison, J. Ellis, M. Sacchi, S.J. Jenkins, B.J. Hinch, *Phys. Rev. Lett.* 106, 186101 (2011).

[2] B.A.J. Lechner, H. Hedgeland, J. Ellis, W. Allison, M. Sacchi, S.J. Jenkins, B.J. Hinch, *Angew. Chem. Int. Ed.* 52, 5085-5088 (2013).

[3] B.A.J. Lechner, M. Sacchi, A.P. Jardine, H. Hedgeland, W. Allison, J. Ellis, S.J. Jenkins, P.C. Dastoor, B.J. Hinch, *J. Phys. Chem. Lett.* 4, 1953-1958 (2013).

[4] P. Rotter, B.A.J. Lechner, A. Morherr, D.M. Chisnall, D. Ward, A.P. Jardine, J. Ellis, W. Allison, B. Eckhardt, G. Witte, *Nat. Mater.*, 15, 397{400 (2016).

ANTON PAAR PRIZE WINNER TALK

LISE-MEITNER-HÖRSAAL

THU03

12:00-12:30

Generation and detection of light in two-dimensional materials

Andreas Pospischil

Vienna University of Technology, Photonics Institute, Vienna, AUT

Two-dimensional (2D) atomic crystals, such as graphene and atomically-thin transition metal dichalcogenides (TMDCs) are currently receiving a lot of attention. The outstanding properties of the 2D material family makes them attractive for a variety of optoelectronic devices. Moreover, the possibility of stacking atomically thin layers on top of each other provides the opportunity to create new "artificial" materials for novel

applications.

Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, shows exceptional electronic and optical properties [1]. The material has been studied extensively during the past years and a vast amount of research has been done to fabricate and characterize photodetectors, mainly for high-speed applications [2]. One drawback of all those photodetectors, which is a consequence of the thinness of only one atomic plane, is the low optical absorption of 2.3 %. One way to overcome this problem is to place a graphene sheet on top of a dielectric waveguide to absorb light not normal to the sheet, but in plane [3]. Therefore, the absorption increases up to 100 %, if the device is made sufficiently long. The waveguide-integrated graphene photodetector operates at all optical telecommunication wavelengths from 1.3 μm to 1.6 μm and exhibits linear response. The bandwidth of the photodetector was measured to be approximately 18 GHz. TMDCs have a layered structure like graphene, but in contrast they are semiconductors with bandgaps in the visible and near-infrared regimes. Here, I will present a p-n junction diode that was realized using an atomically thin layer of tungsten diselenide as channel material [4]. Split gate electrodes introduce doping electrostatically. The diode shows rectifying behavior and operates as a solar energy-harvesting device, if illuminated. Due to the fact that TMDC monolayers are direct bandgap semiconductors, the p-n junction can also be operated as light emitting device. The underlying physical mechanisms leading to light emission in TMDC monolayers are currently not completely understood. Because of high spatial confinement of charge carriers and reduced dielectric screening, excitonic effects play a profound role in this class of materials [5]. I will present temperature and doping dependent photoluminescence measurements, which clarify the interplay between different excitonic states.

[1] Novoselov, K. S. et al. Electric Field Effect in Atomically Thin Carbon Films. *Science* 306, 666–669 (2004).

[2] Koppens, F. H. L. et al. Photodetectors based on graphene, other two-dimensional materials and hybrid systems. *Nature Nanotechnology* 9, 780–793 (2014).

[3] Pospischil, A. et al. CMOS-compatible graphene photodetector covering all optical communication bands. *Nature Photonics* 7, 892–896 (2013).

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[4] Pospischil, A., Furchi, M. M. & Mueller, T. Solar-energy conversion and light emission in an atomic monolayer p-n diode. *Nature Nanotechnology* 9, 257–261 (2014).

[5] Mak, K. F. Tightly bound trions in monolayer MoS₂. *Nature Materials* 12, 207–211 (2012).

COND/NESY

LUDWIG-BOLTZMANN-HÖRSAAL

THU04

13:45-14:00

Sub-threshold measurements of the whispering gallery modes in ring quantum cascade lasers

Martin Holzbauer

Rolf Szedlak, Donald MacFarland, Tobias Zederbauer, Hermann Detz, Aaron Maxwell Andrews, Werner Schrenk, Gottfried Strasser

TU Wien, Vienna, AUT

Quantum cascade lasers (QCLs) are compact coherent light sources for emission of mid-infrared and far-IR radiation [1]. QCLs fabricated into ring cavities have been proven to emit highly collimated beams [2] via the surface/substrate. Another advantage of the ring geometry is the absence of cleaved facets, which allows fabricating very compact resonators. Furthermore, the laser performance is not influenced by the cleave position as for e.g. ridge geometries. For out-coupling of the laser light, a 2nd order distributed feedback (DFB) grating is etched into the upper layers of the waveguide. The feedback is provided by a periodic modulation of the waveguide effective refractive indices. Generally, only small refractive index modulations in the real/imaginary parts are considered in the coupled-mode analysis of Kogelnik and Shank [3]. However, large refractive index steps, by using a Au-semiconductor DFB grating, offer the possibility to couple the antisymmetric modes of the waveguide to surface-plasmon modes [4]. As a result these modes get absorbed by the metal and the symmetric modes are favoured to lase.

We fabricated ring QCLs with metal surface gratings and study the coupling of the modes experimentally and by simulation. A Fourier-transform infrared spectrometer operated in step-scan mode together with a Mercury-Cadmium-Telluride IR-light detector is used to measure the electroluminescence spectrum. The sub-threshold spectrum is recorded as a function of injected current. Below lasing threshold a variety of longitudinal optical modes are visible, which can be identified as the whispering gallery modes in the ring resonator. Above threshold the DFB grating is responsible for selecting a single mode for lasing operation. Furthermore, the sub-threshold gain as a function of photon energy is measured with the Hakki-Paoli technique [5].

- [1] J. Faist, F. Capasso, D.L. Sivco, C. Sirtori, A.L. Hutchinson, and A.Y. Cho, "Quantum Cascade Laser", *Science*, 264 (5158), p. 553-556, 1994
- [2] E. Mujagic, L. K. Hoffmann, S. Schartner, M. Nobile, W. Schrenk, M. P. Semtsiv, M. Wienold, W. T. Masselink, and G. Strasser, "Low divergence single-mode surface emitting quantum cascade ring lasers", *Appl. Phys. Lett.* 93, 161101 (2008)
- [3] H. Kogelnik and C. V. Shank, "Coupled-Wave Theory of Distributed Feedback Lasers", *J. Appl. Phys.* 43, 2327 (1972)
- [4] C. Sigler, J. D. Kirch, T. Earles, L. J. Mawst, Z. Yu, and D. Botez, "Design for high-power, single-lobe, grating-surface-emitting quantum cascade lasers enabled by plasmon-enhanced absorption of antisymmetric modes", *Appl. Phys. Lett.* 104, 131108 (2016)
- [5] B.W. Hakki and T. L. Paoli, "Gain spectra in GaAs double-heterostructure injection lasers", *J. Appl. Phys.* 46, 1299 (1975)

THU05

14:00-14:15

Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites

Menno Bokdam (1)

Tobias Sander (1), Alessandro Stroppa (2), Silvia Picozzi (2), DD Sarma (3), Cesare Franchini (1), Georg Kresse (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Consiglio Nazionale delle Ricerche, L'Aquila, ITA (3) Indian Institute of Science, Bangalore, IND

The development of high efficiency perovskite solar cells has sparked a multitude of measurements on the optical properties of these materials. For the most studied methylammonium (MA) PbI₃ perovskite, a large range (6-55 meV) of exciton binding energies has been reported by various experiments. The existence of excitons at room temperature is unclear. For the MAPbX₃ perovskites we report on relativistic GW-BSE calculations. This method is capable to directly calculate excitonic properties from first-principles. At low temperatures it predicts exciton binding energies in agreement with the reported 'large' values. For MAPbI₃, phonon modes present in this frequency range have a negligible contribution to the ionic screening. By calculating the polarisation in time from finite temperature Molecular Dynamics, we show that at room temperature this does not change. We therefore exclude ionic screening as an explanation for the experimentally observed reduction of the exciton binding energy at room temperature.

THU06

14:15-14:30

Numerical Studies on the Application of Photonic Crystals for EUV mirrors

Ronald Meisels

Friedemar Kuchar

Montanuniversität Leoben, Leoben, AUT

Presently, 193 nm UV radiation is used in lithography. To further reduce the dimensions of electronic components into the sub-10-nm regime the wavelength has to be reduced drastically. A promising option is the use of EUV radiation. A source of particular interest is the Sn plasma produced by laser pulses which emits radiation around 13.5 nm. The use of EUV radiation, however, also presents new challenges. It is no longer possible to simply use the surface of a metal as a mirror. As the EUV lies beyond the plasma frequencies of metals[1] the real part of the dielectric constant ϵ can be < 1 but is no longer negative and therefore the reflection by a single surface is no longer sufficient. It is necessary to use the constructive interference of many interfaces, e.g., alternating layers of Mo and Si are used. This structure can be considered to be a one-dimensional photonic crystal (1D PhC), where the

is very close to unity while Mo is responsible for the needed contrast in ϵ . It is therefore of interest to develop simulation methods to explore more complex PhC structures.

To simulate the reflectivity of an array of different layers, the multiple scattering method (MSM) is used. The scattering of the EUV radiation by each layer is described by a scattering matrix which transforms incident waves into waves propagating away from the layer. Another matrix, the transfer matrix, which is calculated from the scattering matrix, relates the waves incident and travelling away from the layer on one side of the layer with those on the other side. The transfer matrix of a complex system built up of many different layers is the matrix product of the individual transfer matrices. From the corresponding scattering matrix reflectivity and transmissivity of the system are calculated. This method is the basis for the program MULTTEM [2,3] used in the present work. This program can also handle 3D PhCs made of layers containing regular 2D arrays of spheres.

For more general systems the FDTD method[4] has to be used. The reflected field is Fourier transformed and normalized to the Fourier transform of the field propagating in free space. With this method, any type of PhC structure can be investigated.

The feasibility of different materials was investigated for 1D PhCs by calculating the reflectivity of a layer system with Si and another layer with a range of different real and imaginary parts of ϵ . It is found that a large ratio $\text{Re}(\epsilon) / \text{Im}(\epsilon)$ optimizes the reflectivity as long as the number of layers is large enough and the small absorption in Si does not dominate. Comparing with actual values for different elements the highest reflectivities were found for Nb/Si and Mo/Si.

3D PhCs of Mo spheres regularly embedded in Si do not exceed the reflectivity of the 1D layers even for a large number of layers. This is due to the weaker, but still relevant, absorption of the Si matrix. Replacing Si by vacuum, yields reflectivities for small Mo radii exceeding the 1D reflectivities at the expense of reduced bandwidths.

[1] A.D. Rakic, et al., Applied Optics, 37, 5271 (1998).

[2] N. Stefanou, V. Yannopapas, A. Modinos, Comput. Phys. Commun. 113, 198 (1998).

[3] N. Stefanou, V. Yannopapas, A. Modinos, Comput. Phys. Commun. 132, 198 (2000).

[4] K.S. Yee, IEEE Trans. Ant. Prop. 14, 302 (1966).

THU07

14:30-14:45**In-free near infrared lighting from III-nitrides**Dmytro Kysylychyn (1)

Giulia Capuzzo (1), Thibaut Devillers (1), Tian Li (2), Alberta Bonanni (1)

*(1) Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, AUT**(2) Institute of Physics, Polish Academy of Sciences, Warszawa, POL*

Heterostructures based on AlGaN/GaN represent the building blocks of state-of-the-art high-power and optoelectronic devices working in the visible and ultra-violet spectral range. Extending the operation of these systems to other wavelengths, it is expected to open wide prospects for the next generation of devices. We have recently demonstrated room temperature near infrared (NIR) emission originating from Mn-Mg complexes [1,2] in (Al,Ga,Mn) N:Mg. In the perspective of realizing a viable NIR laser structure based on III-nitrides without the need of employing In, we report here on the design, fabrication – by metalorganic vapor phase epitaxy – and characterization of Al (Mn) GaN/GaN distributed Bragg reflectors (DBRs) optimized for the NIR range. The design of the heterostructures is supported by reflectivity simulations based on the transfer matrix method. The critical thickness of the epitaxial AlGaN layers is increased by exploiting the surfactant effect of Mn, obtained by introducing a minimal – i.e. < 0.1% cations – amount of it during the growth [3]. We conclude by showing the enhancement of NIR emission from the DBR structures combined with an (Ga,Mn) N:Mg active layer [4].

The work was supported by the European Research Council (ERC, Project 227690) and by the Austrian Science Foundation (FWF, projects #22477, #24471, #26830).

[1] T. Devillers et al., Scientific Reports 2, 722 (2012).

[2] T. Devillers et al., Appl. Phys. Lett. 103, 211909 (2013).

[3] T. Devillers et al., Crystal Growth & Design 15, 587592 (2015).

[4] D. Kysylychyn, G. Capuzzo, Tian Li, T. Devillers, and A. Bonanni, unpublished data.

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THU08

14:45-15:00

Fabrication of ZnO-based Resonant Tunneling Diodes for Quantum Cascade Structures

Borislav Hinkov (1)

Daniela Ristanic (1), Werner Schrenk (1), Maxime Hugues (2),
Jean-Michel Chauveau (2), Gottfried Strasser (1)

(1) TU Wien, Vienna, AUT (2) CRHEA-CNRS, Valbonne Sophia Antipolis, FRA

1. Introduction

The terahertz (THz) spectral range ($\lambda \sim 30\mu\text{m} - 300\mu\text{m}$) is also known as the “THz-gap” because of the lack of compact semiconductor sources. Various real-world applications would strongly benefit from such devices, like trace gas spectroscopy or security screening. A crucial step for this is the operation of THz-emitting lasers at room temperature. But this seems out of reach with current devices, of which GaAs-based quantum cascade lasers (QCLs) seem to be the most promising ones. They are limited by the parasitic, non-optical LO-phonon transitions (36meV in GaAs), being on the same order as the thermal energy at room temperature ($kT = 26\text{meV}$). One possibility to solve this issue, is the use of larger LO-phonon materials like ZnO (ELO = 72meV). But to master the fabrication of ZnO-based QC structures, a high quality epitaxial growth is crucial followed by a well-controlled fabrication process including (selective) ZnO/ZnMgO etching and depositing low resistance ohmic contacts.

2. Results

Our devices are grown on m-plane [10-10] ZnO-substrate by molecular beam epitaxy (MBE) and patterned by reactive ion etching (RIE) in a CH₄-based chemistry (ICP-power: 200W, RF-voltage: 500V, temperature $\sim 30^\circ\text{C}$, gas-flow: 30/3/3 sccm (CH₄/H₂/Ar), chamber pressure: 20mTorr). The CH₄-process protects the mask by depositing an amorphous carbon-layer and can result in up to infinitely high selectivity towards a resist mask [1]. We tested Au, resist and SiN as masking material, out of which SiN shows the best results, i.e. vertical sidewalls for 10 μm of ZnO etching, a selectivity of well above 1:30 and an etch-rate of 62nm/min. The slightly rough surface of the etched ZnO is smoothed by an additional wet etching in diluted H₃PO₄. In a first experiment we measured the current-voltage characteristic of 50 μm to 150 μm square mesas for

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a reference RTD structure, i.e. a structure that contains a 30nm undoped ZnO layer sandwiched between two 200nm thick contact layers (n-doped $5 \times 10^{18} \text{cm}^{-3}$). The doping is continuously altered between the two sections over 50nm. We extract contact resistances of $8 \times 10^{-5} \text{W cm}^2$, which are in good agreement with literature. The electron mobility is above $100 \text{cm}^2/\text{Vs}$. This value is one order of magnitude lower than literature values. We believe it is due to a parasitic, low quality layer at the growth interface or due to a bad quality of the substrate. Next steps will be to fabricate real RTD structures on high quality substrates, to prove that resonant electron tunneling can be achieved in ZnO as one important building block of a QCL.

[1] S.-W. Na, M. H. Shin, Y. M. Chung, J. G. Han, and N.-E. Lee, "Investigation of process window during dry etching of ZnO", J. Vac. Sci. Technol. A 23, 898 (2005).

THU09

15:00-15:15**Exciton binding energies and lifetimes in atomically thin layered semiconductors**

Kerstin Hummer

Juraj Mavracic

Faculty of Physics, University of Vienna, Vienna, AUT

The achievements in the fabrication of atomically thin layered materials [1] have enabled explorations of novel physical properties exclusively inherent to low dimensional structures. Similar to graphene, atomically thin layers of transition metal dichalcogenides (TMX₂) can be prepared. Among them, the group-6 materials with its prototype molybdenum disulfide (MoS₂) have attracted intense interest because of its distinct electronic, optical and catalytic properties [3]. Triggered by these outstanding properties, monolayer MoS₂ has been proposed as semiconducting analogue of graphene with several potential applications [4-6]. The latest innovation in this research field is the vertical and lateral stacking of different (semi) conducting layers designing so-called Van der Waals heterostructures with desired physical properties [7]. Apart from TMX₂, some group-13 monochalcogenides (MX; M = Ga, In

and X=S, Se, Te) also crystallize in layered, hexagonal bulk structures. These are in focus of the present study. In particular, monolayers of these materials are currently under investigation, since they have been suggested as potential photocatalysts for water splitting [8], i.e. a promising method for solar energy conversion by sunlight induced hydrogen reduction combined with an oxidation reaction producing H₂ and O₂. Important electronic and optical properties that determine whether the material is a suitable photocatalyst are: (i) the magnitude of the optical gap, (ii) the band off-set of the valence band maximum and the conduction band minimum with respect to the oxidation potential of H₂O and the reduction potential of H⁺, respectively, (iii) the exciton binding energies, and (iv) the excitation lifetimes.

In the current work, we address these issues with particular emphasis on the single- and double-layers and present computational results based on density functional theory (DFT) [9] obtained using the Vienna Ab initio Simulation Package (VASP) [10]. An accurate description of the electronic and optical properties including the electron-hole interactions has been achieved by performing quasiparticle calculations within the GW approximation [11] and solving the Bethe-Salpeter equation [12].

- [1] K. S. Novoselov et al., Proc. Natl. Acad. Sci. 102, 10451 (2005)
- [2] C. Ataca et al., J. Phys. Chem. C 116, 8983 (2012) ; S. Lebègue et al., Phys. Rev. X 3, 031002 (2013)
- [3] G.-B. Liu et al., Chem. Soc. Rev. 44, 2643 (2015) ; H. Zeng and X. Cui, *ibid.*, 2629; H. L. Zhuang and R. G. Hennig, J. Phys. Chem. C 117, 20440 (2013)
- [4] B. Radisavljevic et al., Nature Nanotech. 6, 147 (2011)
- [5] T. Heine, Acc. Chem. Res. 48, 65-72 (2015) ; D. Lembke, S. Bertolazzi, and A. Kis, *ibid.*, 100 (2015)
- [6] T. Cao et al., Nat. Commun. 3, 887 (2012) ; H. Zeng et al., Nat. Nanotechnol. 7, 490 (2012)
- [7] A. K. Geim and I. V. Grigorieva, Nature 499, 419 (2013) ; P. Rivera et al., Nat. Commun. 6: 6242 doi: 10.1038/ncomms7242 (2015)
- [8] Y. Ma et al., Phys. Chem. Chem. Phys. 15, 7098 (2013) ; H. L. Zhuang and R. G. Hennig, Chem. Mater. 25, 3232 (2013)
- [9] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999)
- [10] G. Kresse and J. Furthmüller, J. Computat. Mater. Sci. 6, 15 (1996) ; Phys. Rev. B. 54, 11169 (1996)

[11] M. Shishkin and G. Kresse, Phys. Rev. B 74, 035101 (2006) ; id. Phys. Rev. B 75, 235102 (2007)

[12] T. Sander, E. Maggio, and G. Kresse, Phys. Rev. B 92, 045209 (2015)

THU10

15:45-16:00**Universal criterion for designability of heteropolymers**Chiara Cardelli (1)

Valentino Bianco (1), Lorenzo Rovigatti (2), Christoph Dellago (1), Ivan Coluzza (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Rudolph Peierls Centre for Theoretical Physics Oxford University, Oxford, GBR

Heteropolymers are important examples in material science of self-assembling systems. The technology for the synthesis and manipulation of such heteropolymers is already advanced [1], and it is nowadays possible to synthesize polymers made of up to 7 different monomers with complex pattern arrangements (e.g. block copolymers). However, it is still not possible to design heteropolymers with control over the single chain self-assembling properties comparable to what natural biopolymers, such as DNA and proteins, can achieve. Here we introduce a criterion to discriminate between polymers that can be designed to adopt a predetermined structure from polymers that cannot, and show that this criterion is fulfilled by the addition of few directional interactions to the monomers of the chain. The criterion is based on the appearance of a particular peak in the radial distribution function that dominates over the random packing of the heteropolymer. We show that the presence of such a peak indicates that it exists at least one pattern of building blocks that will drive the system to collapse towards a specific target structure. Moreover, we show that the peak is a universal feature of all designable heteropolymers, as it is dominating also the radial distribution function of natural proteins. The criterion that we present can be applied to engineer new types of self-assembling modular polymers that will open new applications for polymer-based materials science.

[1] T. P. Lodge, Macromolecular Chemistry and Physics 204, 265 (2003).

THU11

16:00-16:15

Star - long chain mixtures: a novel coarse-graining approach

Emanuele Locatelli

Barbara Capone, Christos N. Likos

Faculty of Physics, University of Vienna, Vienna, AUT

We present a novel multi-scale coarse graining approach, suitable for mixtures of long chains and star polymers. The approach is based on a multi-blob description of the long chain, where each blob, representing N_0 monomers, interact with the star polymer through an effective potential. Such effective interaction has been first calculated numerically for star polymers of different functionality $50 < f < 150$ and different arm length $50 < N < 150$. Through a theoretical analysis of the numerical results, we provide an approximate, analytical form for the interaction potential, valid for stars of arbitrary functionality and arbitrary size. We test our approach, comparing the effective interaction between a star polymer and a long chain of length N_c , at both coarse-graining and monomer-resolved level. We find that the coarse-graining approach yields an excellent agreement with respect to monomer-resolved results.

THU12

16:15-16:30

Influence of cross-links coordination on the mechanical behavior of polymeric structures

Huzaifa Shabbir

Markus Hartmann

Faculty of Physics, University of Vienna, Vienna, AUT

(Reversible) cross-linking is a common strategy to specifically tailor the mechanical properties of natural and synthetic polymeric systems. In biological materials, cross-links are often weaker than the covalent bonds holding the structure together. Thus, upon loading these bonds rupture before the covalent backbone fails, providing an efficient energy dissipation mechanism. Furthermore, the reversibility of the cross-links provides the material with a self healing mechanism because

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broken cross-links may reform after release of the load. In the context of biological materials such cross-links are often called “sacrificial bonds” and they can be found in a large variety of structures like bone, wood, silk and the mussel byssus [1].

While the coordination of cross-links (i.e. the number of monomers participating in one cross-link) often varies in real systems (e.g. depending on pH the Fe-DOPA complex in the mussel byssus is known to exist in the mono-, bis- and tris-state), theoretical and simulation work dealing with the effect of cross-links on the mechanics of polymeric structures (aligned fiber bundles and random polymer networks) mostly investigate the effect of two fold coordinated cross-links only. In the current study, we aim at closing this gap by explicitly investigating the mechanical response of a polymeric system as a function of the coordination of reversible cross-links.

In the study presented, the Monte Carlo method is used to investigate the mechanical properties of cross-linked polymeric systems. The coordination of cross-links is controlled using the framework given by potentials of the REBO (Reactive Empirical Bond Order) type. In these potentials, the strength of an individual bond depends on the coordination of the involved atoms. The current study investigates the effect of different cross-links coordination on the mechanical properties of polymeric systems including random fiber networks and aligned fiber bundles. We present computational loading experiments performed at different cross-links densities and different spatial arrangement of cross-links and discuss the most important mechanical properties (stiffness, strength and toughness). As previous work on two-fold coordinated cross-links was showing a strong dependence of the mechanical performance on the topology of formed cross-links [2-4], in the present investigation special emphasis is put on the interplay of topology and mechanics.

[1] Fantner et al., *Biophysical Journal* 90, 1411 (2006)

[2] Nabavi et al., *New Journal of Physics* 16, 013003 (2014)

[3] Nabavi et al., *Bioinspired, Biomimetic and Nanobiomaterials* 3, 139 (2014)

[4] Nabavi et al., *Physical Review E* 91, 032603 (2015)

THU13

16:30-16:45

Stability of carbon nanotubes under hydrostatic pressure investigated by Monte Carlo simulations

Markus Hartmann

Faculty of Physics, University of Vienna, Vienna, AUT

Carbon nanostructures are a fascinating class of materials combining high stiffness with low weight and exceptional toughness that makes carbon a promising candidate for applications in structural mechanics. Understanding the mechanical properties of these structures on every length scale is of utmost importance to be able to exploit the full potential of these materials. Monte Carlo simulations are a perfect tool to gain an insight into the complex deformation behavior of carbon nanostructures like graphene [1], nanotubes [2] and fullerenes [3] on an atomic scale. In the presented work I will present investigations on the mechanical stability of carbon nanotubes under hydrostatic pressure. Carbon nanotubes of different sizes and chiralities will be investigated. The shape of the initially circular cross-section of the tubes will be monitored. Under increasing load it first ovalizes into an elliptic shape, upon further increase of the load the shape further evolves into a peanut-like shape. Finally I will discuss the reversibility of the shape change when the applied load is reduced.

[1] Hartmann et al., Europhys. Lett. 103, 68004 (2013)

[2] Sun et al., Proc. Appl. Math. Mech. 13, 7 (2013)

[3] Holec et al., Phys. Rev. B 81, 235403 (2010)

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THU14

16:45-17:00**Studying the interaction of filled SWCNTs with NO₂**Filippo Fedi (1)

Oleg Domanov (1), Hidetsugo Shiozawa (1), Paola Ayala (1), Kazuhiro Yanagi (2), Andrea Goldoni (3), Paolo Lacovic (3), Silvano Lizzit (3), Elena Magnano (3), Silvia Nappini (3), Igor Pís (3), Thomas Pichler (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Department of Physics, Tokyo Metropolitan University, Tokyo, JPN (3) Elettra Sincrotrone Trieste, Basovizza - Trieste, ITA

Controlling the interaction between gases and Single Wall Carbon Nanotubes (SWCNTs) is a key point for sensors made with nano-carbons [1]. Here we present the latest progress on the understanding of the interaction between nitrogen dioxide and metallicity-sorted ultra-pure SWCNTs filled with Ni and Fe [2]. The effect of the different gas dosing on the SWCNTs was measured using UPS, XPS and XAS carried out at SUPERESCA beamline in ELETTRA. The interaction with gas is recognized in the core levels, valence bands and transport measurements. Gas desorption at room temperature was observed, followed by major change in the density of states at the Fermi level. The innovative results help us to get highest selectivity and sensitivity for gas sensing at room temperature. We acknowledge the financial support by FWF, EU.

THU15

17:00-17:15**Magnetic molecules arranged in carbon nanotubes**Oleg Domanov (1)

Markus Sauer (1), Michael Eisterer (2), Takashi Saito (3), Herwig Peterlik (1), Eugen Weschke (4), Jacek Osiecki (5), Karina Schulte (5), Thomas Pichler (1), Hidetsugo Shiozawa (1)

(1) University of Vienna, Vienna, AUT (2) TU Wien, Vienna, AUT (3) National Institute of Advanced Industrial Science and Technology, JPN (4) Helmholtz-Zentrum Berlin, Berlin, GER (5) MAX IV Laboratory, Lund University, Lund, SWE

Metal-organic molecular magnets are of great interest because of their unique magnetic properties. These arise from interactions between the

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molecular compounds in the confined nanospace of single-wall carbon nanotubes (SWCNT), forming one-dimensional structures. We study the magnetic, electronic and structural properties of such molecular chains by means of X-ray/UV Photoemission Spectroscopy (XPS, UPS), X-ray Absorption Spectroscopy (XAS), X-ray magnetic circular dichroism (XMCD), XRD and SQUID. XRD data analyzed with the Rietveld method suggests that the intermolecular spacing of the chains is dependent on the nanotube diameter. We discuss magnetic ground states, superparamagnetism and possible bulk magnetic ordering of this system as well as the effect of electron doping by potassium intercalation. Our work provides interesting insight into the properties of 1D molecule chains that would pave the way towards advanced molecule-based magnets.

[1]M.Kharlamova et al. *Nanoscale* 7, 1383 (2015).

[2]A.Briones-Leon et al. *Phys. Rev. B* 87, 195435 (2013).

[3]H.Shiozawa et al. *Scientific Reports* 5, 15033 (2015) Weacknowledge financial support from the Austrian Science Fund (FWF, p27769-N20).

FAKT

LISE-MEITNER-HÖRSAAL

THU16

13:45-14:00

Simulations of deexcitation to ground state in a beam of antihydrogen generated in the ASACUSA double CUSP trap

Hans Spitzer

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT

The ASACUSA experiment tries to find matter-antimatter asymmetries by aiming at measuring the hyperfine structure of antihydrogen with a similar degree of precision as it is known for hydrogen. As production of antihydrogen still is a very complex task and available quantities are limited, software tools based on the particle physics toolkit geant4 have been built and are currently being extended to simulate the

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antihydrogen processes in the ASACUSA beamline. This should enable better assessment under which conditions (beam energy, strengths of magnetic and electric fields) a high share of ground state antihydrogen atoms can be achieved in the spin flip cavity for optimal measurement of the resonance frequency. The status of the further development of the simulations and the software will be the topic of this talk.

THU17

14:00-14:15

Progress report of the ASACUSA Hbar HFS experiment

Volkhard Mäckel

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT

The ASACUSA collaboration at the Antiproton Decelerator of CERN aims at a precise measurement of the ground-state hyperfine splitting (GS-HFS) of antihydrogen, which promises to be one of the most sensitive tests of CPT symmetry. Shortly, an antihydrogen beam will be produced, and the GS-HFS determined in a Rabi type experiment [1]. The GS-HFS will be driven using a spin-flip resonator cavity, and the spin state analyzed with a superconducting sextupole magnet, which focuses the spin flipped atoms out of the beam. The remaining atoms are then counted with a dedicated detector, consisting out of a BGO detector and a hodoscope.

In my presentation, I will give an overview of the current status of the ASACUSA, as well as the achievements made during the antiproton run this year at CERN.

[1] E. Widmann et al., *Hyperfine Interactions* 215, 1 (2013).

THU18

14:15-14:30

GERDA - the search for neutrinoless double beta decay

Peter Grabmayr

Physikal. Institut, Universität Tübingen, Tübingen, GER

The GERDA (GERmanium Detector Array) experiment searches for the neutrinoless double beta decay of ^{76}Ge . The neutrinoless double beta decay is a lepton number violating process and if observed would prove the Majorana nature of the neutrino. It then would lead to physics beyond the Standard Model. GERDA is located at the Laboratori Nazionali del Gran Sasso of INFN and operates enriched Ge detectors directly in liquid argon. The liquid argon acts not only as cooling medium, but also as passive (Phase I) or active (Phase II) shield against external radiation.

After a successful completion of GERDA Phase I in 2013, that resulted in a lower limit on the half-life of $^{76}\text{Ge} > 2.1 \cdot 10^{25}$ yr (90 % C.L.) the experiment was upgraded to double the target mass and significantly reduce the background level. Newly designed Ge detectors were installed along with a veto system detecting the liquid argon scintillation light. Results from Phase I, expectations from present data and competitors will be discussed.

THU19

14:30-14:45

PERC - A Status Report

Erwin Jericha

Atominstytut, TU Wien, Vienna, AUT

With this presentation we will give the latest update on the development of the PERC facility, dedicated to the high-precision study of neutron beta decay.

THU20

14:45-15:00

Measuring the Hydrogen Ground State Hyper-Fine Splitting through the p1 and s1 transition

Sergio Arguedas Cuendis

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT; on behalf of the ASACUSA collaboration

The ASACUSA collaboration is aiming to measure the ground state hyperfine structure of antihydrogen to test the CPT symmetry. In context of this experiment a hydrogen source is used to characterize several components of the antihydrogen spectroscopy setup.

This contribution will give a detailed explanation of the cavity, on the principles of this Rabi-type beam spectroscopy experiment with a focus on the physics behind the spin-flip driving cavity. Measuring a π_1 or σ_1 transition depends on the direction of the oscillating magnetic field with respect to the static magnetic field. Modifications were made in the cavity, in order to allow for a flexible switching between the two types of transitions. Currently the modified cavity is installed at the hydrogen beam setup and first resonance spectra taken in the Earth's magnetic field environment are expected to be seen this summer. Finally, the plans for a future measurement with a cavity shielding so that a better static magnetic field is obtained will be mentioned.

THU21

15:00-15:15

ASACUSA Atomic Hydrogen Beam Line

Markus Wiesinger

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT; on behalf of the ASACUSA collaboration

Spectroscopy of the hyperfine transitions of ground state anti-hydrogen provides a test of CPT symmetry. An atomic hydrogen beam line at CERN is used to commission the spectroscopy instruments for measurements of the ground state hyperfine transitions in anti-hydrogen. An overview of the beam line will be given, with focus on newly installed analyzer magnets and a method for velocity selection. One analyzer magnet consists of 12 rectangular permanent magnets in a Halbach configuration supported by a 3d-printed mount. A characterization of the magnetic field of 5 of the installed magnets will be presented. Furthermore, velocity selection using the two polarizing permanent sextupole magnets with variable distance will be shown.

THU22

15:45-16:00

Full reconstruction of Bs meson decays at Belle

Felicitas Andrea Breibeck

HEPHY, Austrian Academy of Sciences, Vienna, AUT

Besides its great success the Standard Model of Particle Physics is known to be incomplete. Thus physicist are searching for physics beyond the Standard Model. Leptonic B_s meson decays such as $B_s \rightarrow \tau^+ \tau^-$ are very sensitive to new physics. However, as there are neutrinos in the final state, the reconstruction of such decay modes is very challenging due to the information loss regarding momentum and energy of the neutrino resulting in high combinatorial background as only limited kinematic constraints can be applied during the B_s reconstruction. The Belle experiment located at the KEKB collider in Tsukuba, Japan, has collected a data sample of 121fb^{-1} at the $\Upsilon(5S)$ resonance with a center-of-mass energy of 10.87 GeV, which corresponds to approximately 7.1 ± 1.3 million B_s meson pairs. An analysis method, the so-called hadronic tagging, opens the possibility to study B_s decays with neutrinos in the final state at Belle. The main task of this hadronic tag is to fully reconstruct one of the two produced B_s mesons in a hadronic final state. Thus, the kinematic of the second B_s meson becomes accessible applying energy and momentum conservation and the combinatorial background is significantly reduced as all detected charged tracks and energy clusters used in the hadronic tag are eliminated for the reconstruction of the signal side B_s .

In this talk we present the recently developed B_s hadronic tag for the Belle experiment, its software architecture and the prospects it opens for future Belle analyses. The method used in this software tool is based on a hierarchical approach in which the B_s mesons and their daughters are reconstructed in several stages. Instead of simply relying on selections applied to kinematic variables or mass distributions, we train neural networks for every implemented decay mode in every stage of the hadronic tag. Thus, more than 100 neural networks provide a powerful discrimination between correctly reconstructed B_s candidates and background events.

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THU23

16:00-16:15**Resonant Λ_c to Sigma pi pi decays in Belle data**Manfred Berger (1)

Ken Suzuki (1), Christoph Schwanda (2), Felicitas Breibeck (2), Robin Glattauer (2)

(1) Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT (2) HEPHY, Austrian Academy of Sciences, Vienna, AUT

The $\Lambda(1405)$ resonance can be described as KN a meson-baryon quasi bound state strongly coupled to $\Sigma\pi$. The KN reaction around the threshold is reasonably well constrained. However, the $\Sigma\pi$ amplitude is still afflicted with large uncertainty. In light of this a method, analogue to Cabibbo's extraction of the pion scattering length from a cusp occurring at threshold in the $\pi\pi$ spectrum from kaon decays, has been proposed for the weak $\Lambda_c \rightarrow \Sigma\pi\pi$ decay. Pursuing this approach at the Belle experiment leads to a high purity data sample of $\Sigma^+\pi^+\pi^-$, $\Sigma^0\pi^+\pi^0$ and $\Sigma^+\pi^0\pi^0$ decay modes, allowing both a measurement of branching ratios relative to $pK^+\pi^+$ and a direct measurement of intermediate resonances. In this report we give preliminary results for these measurements.

THU24

16:15-16:30**Quality Assurance and Data Analysis for the Belle II Silicon Vertex Detector**Lukas Bulla*HEPHY, Austrian Academy of Sciences, Vienna, AUT*

The Institute of High Energy Physics (HEPHY), which belongs to the Austrian Academy of Sciences (OAW), is participating in the Belle II experiment. The major task is to develop and construct the Silicon Vertex Detector (SVD) which is an inner detector of Belle II. As frontier B-physics experiments, such as Belle II, require that the SVD is a technically highly advanced detector and unique in its construction and scope of application. Therefore ongoing tests on functionality and quality assurance have to be conducted. These tests comprise in-house

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small-scale ladder checks to high energy particle beam tests. This talk should give a brief overview about data analysis from single ladders to fully configured telescope tests and the developed test environment. Thus the talk contains signal analysis and first tracking tests with a fully assembled L5 ladder in the final SVD configuration at CERN-SPS and DESY as well as the development of a Ladder-Test-System (LTS). The LTS aimed at testing the functionality of the fully assembled ladder with a ^{90}Sr source. Moreover, an open CO_2 cooling device (ACBC) was developed for cooling tests after mounting the ladders on the final setup.

THU25

16:30-16:45

Performance simulation of the Barrel Scintillator Tile Hodoscope for PANDA

Dominik Steinschaden (1)

Lukas Gruber (1), Marius Chirita (1), Ken Suzuki (1), Gamal Ahmed (3)

(1) Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT (2) Al-Azhar University, Faculty of Science, Physics Department, Cairo, EGY

The PANDA experiment, currently under construction at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany, addresses fundamental questions in hadron and nuclear physics via interactions of antiprotons with nucleus/nuclei. The High Energy Storage Ring will provide an antiproton beam with a momentum range of 1.5 – 15 GeV/c and an average collision rate on the fixed target of 20 MHz is envisaged. The barrel-shaped scintillator tile hodoscope, covering the central region of the detector, will be one of the key components to determine the time origin of the tracks and provides particle identification for slow particles below 700 MeV/c. To achieve a time resolution < 100 ps plastic scintillator tiles with minimum material budget read out by Silicon Photomultiplier (SiPM) have been selected.

In this presentation the performance of the particle identification and event separation based on the barrel scintillator tile hodoscope will be discussed.

THU26

16:45-17:00**Search for Stop Pair-Production in the Single-Lepton Channel in Supersymmetry Models with Highly-Compressed Spectra with the CMS Detector at the LHC**Mateusz Zarucki*HEPHY, Austrian Academy of Sciences, Vienna, AUT*

This search focuses on models of Supersymmetry where the mass gap between the lightest top squark (supersymmetric partner of the top quark) and the lightest supersymmetric particle (LSP) is smaller than the W boson mass, a scenario that is motivated by naturalness and dark matter constraints. The signal events consist of top squark pair-production followed by 4-body decays into a lepton-neutrino (quark-antiquark) pair, a b quark and the LSP. The LSPs and the neutrino escape the detector, leading to a missing transverse energy signature. Compressed regions are a challenging sector of parameter space to study, as the visible decay products have low momentum and generally do not pass detector acceptance thresholds, however, this difficulty can be mitigated by the system being boosted by initial-state radiation (ISR). The results from the CMS Experiment at the Large Hadron Collider (LHC), CERN, are presented.

THU27

17:00-17:15**Search for the rare decay $B_s^0 \rightarrow \tau^+ \tau^-$ at Belle**Lukas Gosch

Felicitas Andrea Breibeck

HEPHY, Austrian Academy of Sciences, Vienna, AUT

In the Standard Model of particle physics (SM) the branching ratio of the decay $B_s^0 \rightarrow \tau^+ \tau^-$ is predicted to be about $9 \cdot 10^{-7}$. However, physics beyond the SM can significantly increase this value by orders of magnitude. The SM is known to be incomplete and leaves open questions regarding e.g. mixing angles, hierarchy of particle masses and dark matter.

The aim of this work is to search for and obtain the first direct experimental information on the decay $B_s^0 \rightarrow \tau^+\tau^-$. No direct experimental information is currently available as this decay is nearly impossible to reconstruct in hadronic collider experiments due to the neutrinos in the final state.

In this talk we present a reconstruction mechanism and its efficiency for the $B_s^0 \rightarrow \tau^+\tau^-$ decay in asymmetric energy e^+e^- collisions recorded by the Belle experiment at the the $\Upsilon(5S)$ resonance corresponding to a center of mass (c. m.) energy of 10.87 GeV.

We use the information of one fully reconstructed neutral B_s^0 meson, the so called hadronic tag, and seek evidence for the signal decay in the rest of the event. The decay products of the hadronic tag are removed from the event and the signal- B_s^0 characteristics are sought among the remaining particles. Signal events are required to be consistent with each τ decaying to a single charged particle and one or two neutrinos, namely $\tau \rightarrow e\nu\nu'$, $\mu\nu\nu'$, $\pi\nu$, $\rho\nu$, with ρ decaying to $\rho \rightarrow \pi\pi^0$. Dominant background is being suppressed by vetoing events with identified charged kaons K^+ or reconstructed $K_s^0 \rightarrow \pi^+\pi^-$ particles on the signal-side. Variables that are expected to have a strong discriminant power are e.g. the residual energy in the electromagnetic calorimeter and the missing mass of the reconstructed event.

MBU**CHRISTIAN-DOPPLER-HÖRSAAL****THU28****13:45-14:15****Digital Aberration Correction for in-vivo Cellular Retinal Imaging**Rainer Leitgeb*Medical University of Vienna, Vienna, AUT*

Optical Coherence Tomography (OCT) has already become an indispensable tool in precise retinal diagnostics. Modern systems

provide micrometer resolution in combination with high imaging speed to record full volumes within one second and less. Still, its resolution is limited by strong aberrations due to the in general poor optical quality of the ocular media, such as the cornea and the lens. Translating adaptive optics technology from astronomy to ophthalmoscopy allows correcting for those aberrations in the human eye yielding cellular resolution details. Those techniques are however expensive and difficult to combine with OCT. Recent developments applied techniques from holography to correct for aberrations in post-processing, by making use of the complex field information that is available in OCT. However, for in-vivo imaging, the field information suffers from motion induced phase distortion. Only high-speed recording employing parallel sensing achieves sufficient lateral phase correlation to allow for wavefront reconstruction and subsequent digital aberration correction. We present the method of digital aberration correction that does not need any additional setup input parameters, and is iteration free. We further demonstrate in-vivo retinal photoreceptor imaging by employing the technique to high-speed line field OCT data recorded at 2000 tomograms/sec. High-resolution retinal imaging is expected to gain increasing importance with the advent of cellular treatment and repair techniques as well as gene therapy.

THU29**14:15-14:30****Designing highly specific probes with tunable affinity**Francesca Nerattini

Luca Tubiana, Ivan Coluzza

Faculty of Physics, University of Vienna, Vienna, AUT

Finding ligands able to bind with high specificity to a target protein is one of the major challenges in medical research, especially for the development of anti-cancer drugs[1]. Recently it was shown that therapies based on nanoparticles are ineffective[2] due to the difficulty of designing a particle coating which specifically recognizes cancerous cells. We aim at developing a novel computational protocol, based on the recently developed caterpillar[3] coarse grained model, to design proteins that can be used as effective coatings for novel cancer

targeting nanoparticles. Key to the success of the targeting are proteins, which are highly selective towards the receptors on the cell membrane but with tunable binding affinity to reduce binding to healthy cells[4]. According to previous studies[5], performed with lattice protein models, such special protein sequences can be obtained by introducing destabilizing mutations in proteins designed to strongly bind to a target substrate. Since such control has not been attempted before on real proteins, we test the feasibility of our approach on a reference system first. We present results of our preliminary studies for a “protein like” pocket. First we design the sequences of both protein and pocket at the same time, in order to optimize the protein-ligand interactions. Then we monitor the binding affinity as a function of the percentage of destabilizing mutations in the amino-acids sequence of the protein.

[1] Dubacheva, Galina V., et al. Proceedings of the National Academy of Sciences 112.18 (2015): 5579-5584.

[2] Wilhelm, Stefan, et al. Nature Reviews Materials 1 (2016): 16014.

[3] Coluzza, Ivan. PloS one 6.7 (2011): e20853.

[4] Martinez-Veracochea, Francisco J., and Daan Frenkel. Proceedings of the National Academy of Sciences 108.27 (2011): 10963-10968.

[5] Coluzza, Ivan, and Daan Frenkel. Biophysical journal 92.4 (2007): 1150-1156.

THU30

14:30-14:45

The role of water in the selection of stable proteins at ambient and extreme thermodynamic conditions

Valentino Bianco (1)

Giancarlo Franzese (2), Christoph Dellago (1), Ivan Coluzza (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) University of Barcelona, Barcelona, ESP

Natural evolution selects proteins that are functional under particular environmental conditions. Here we study, using computer simulations, how water contributes to this selection process. We follow the idea of the protein design, which artificially optimizes amino acid sequences aiming at a unique folded state under specific thermodynamic conditions. First, we introduce a novel selection protocol for

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sequence-optimization, which is efficient at both ambient and extreme thermodynamic conditions. Thanks to the computational efficiency of the model we are able to assess the stability of artificial proteins for a wide range of pressures and temperatures and for a series of protein structures, comparing all the results for different design strategies. We are able, for the first time, to make a comprehensive study of the region where protein design is possible, and compare it with the natural borders where active stable proteins are observed. In particular, we show that sequences optimized at high temperature are stable in a temperature-pressure range considerably broader than proteins selected at ambient and low temperature. We find that these super-stable sequences are characterized by an optimized segregation between the hydrophilic surface and the hydrophobic core, comparable to the one observed in many natural proteins. Moreover, we demonstrate that sequences with an extreme hydrophobic/hydrophilic separation are less stable than the super-stable sequences. This means that an optimal segregation level exists, allowing the protein to have partially hydrophobic surfaces. Such an exposure is not a compromise between stability and biological functionality of the proteins, but rather a natural consequence of the water properties. Our results elucidate the evolutionary pressure exercised by water on the hydropathy profile as function of the thermodynamic state point, with implications for the understanding of natural and artificial selection of proteins at ambient and extreme conditions.

THU31

14:45-15:00**Modeling of Asymmetric Model Vesicles: Joint Refinement of SANS and SAXS Data**Barbara Eicher (1)

Drew Marquardt (1), Frederick A. Heberle (2), Milka Doktorova (3), John Katsaras (2), Georg Pabst (1)

(1) Institute of Molecular Biosciences, Biophysics Division, University of Graz, Graz, AUT (2) Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA (3) Department of Physiology and Biophysics, Weill Cornell Medical College and the Tri-Institutional Training Program in Computational Biology and Medicine, New York, USA

Mammalian plasma membranes consist of an asymmetric lipid distribution along the two leaflets, in other word the inner leaflet is compositional different from the outer. The asymmetry of the bilayer is expected to affect various membrane properties, such as membrane potential, permeability, surface charge, and stability. Bilayer asymmetry is also hypothesized to affect structural properties of the membrane, like bilayer thickness and thickness of the single leaflets for example. However, due to the difficulty of preparing asymmetric vesicles the majority of model membrane studies have been performed on symmetric bilayers, where inner and outer membrane leaflets are identical in composition. Of recent, we developed new protocols for the construction and characterization of asymmetric vesicles amiable for scattering and NMR experiments with a well-defined inner and outer leaflet composition. Quantification of bilayer composition and degree of asymmetry enables the determination of transverse structural parameters, such as, area per lipid and the bilayer thicknesses of the various phases in each leaflet. We are able to determine these structural parameters through a joint analysis of small angle neutron scattering (SANS) data exploiting D/H contrast variation and small angle X-ray scattering (SAXS). Here we report on the first probe-free analysis yielding insights into a transbilayer coupling mechanisms. First results have shown a decrease in lipid packing density at room temperature of the DPPC-rich phase (outer leaflet) compared to typical gel phase packing, indicating a disordering effect from coupling to the fluid inner leaflet. Further, our analysis of fluid DPPC/POPC asymmetric vesicles revealed that inner and outer membrane layers are not coupled to each other. This work is supported by the Austrian Science Fund FWF, Project No.P27083-B20 (to G.P.).

THU32

15:00-15:15

EBIS charge breeder for 2nd generation hadron therapy facilities

Johanna Pitters

CERN, Geneva, SUI

Recent developments in hadron therapy aim to include radioactive beams for simultaneous treatment and diagnostics. In parallel, as an

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alternative to synchrotron-based facilities, new linac-based accelerator concepts are under consideration, like CABOTO, the Carbon Booster for Therapy in Oncology. Both approaches require a highly efficient charge breeding scheme beyond the capabilities of the commonly used ECR ion source. A potential candidate is a charge breeding scheme based on an Electron Beam Ion Source. At CERN a new electron gun, the MEDeGUN, was designed specifically for rapid charge breeding of C6+ ions to be used in linac-based therapy facilities.

In this talk potential schemes for hadron therapy using 11C will be discussed and a status report on MEDeGUN will be given.

THU33

15:45-16:00

Long-term study of New Particle Formation (NPF) events as a source of Cloud Condensation Nuclei (CCN) concentrations in the urban background of Vienna

Maria del Carmen Dameto de Espana

Anna Wonaschütz, Gerhard Steiner, Regina Hitzenberger

Faculty of Physics, University of Vienna, Vienna, AUT

Atmospheric aerosols have profound impacts on global climate directly by scattering and absorbing solar radiation and indirectly by modifying and altering cloud properties. The indirect aerosol effects occur due to aerosol particles acting as cloud condensation nuclei (CCN) and as ice nuclei. They constitute the largest uncertainty in estimating the aerosol radiative forcing and global climate change. In order to better quantify the global CCN budget, it is necessary to determine the sources responsible for atmospheric CCN. Observations and model studies (e.g. Kerminen et al., 2012) have demonstrated that New Particle Formation (NPF) events can be an important source of CCN in the atmosphere. Only few studies (e.g. Asmi et al., 2011), however, have linked observed NPF and growth events directly to increases in measured CCN concentrations. Most of these studies were performed in remote or background locations. There is a lack of continuous long-term parallel measurements of CCN concentrations and of NPF events in urban aerosols. In order to provide more information about NPF events as a possible source of CCN, a long term study was done from June 2014 to December 2015 in

the urban background of Vienna Measurements of size distributions and CCN concentrations are performed at the aerosol laboratory located on the roof (35m above ground) of the Physics building of the University of Vienna in central Vienna.

A CCNC (Cloud Condensation Nuclei Counter) designed at the University of Vienna and operating on the principle of a static thermal diffusion chamber (Giebl et al., 2002), was used to measure CCN concentrations and activation ratios at low supersaturations (0,5%). NPF events were identified in a continuous size distribution dataset measured with a Vienna-type DMPS (Differential Mobility Particle Sizer, Winklmayr et al., 1991) and a SMPS 3082 (TSI, Inc.). NPF event and non-event days are classified using the criteria of Dal Maso et al. (2005).

NPF events and the continuing growth of the newly-formed particles are sometimes superposed by local pollution plumes. Traffic emissions could additionally increase the concentration of CCN-active particles during a NPF event. A Multi Angle Absorption Photometer (MAAP) measuring black carbon concentrations is therefore used to monitor the contribution of traffic emissions and local pollution plumes to the aerosol at the station. Weather conditions during NPF events were also taken into account. For this study, events and CCN concentrations were considered only when weather conditions and black carbon concentrations stayed constant before, during and after the event.

The results indicate that in some cases NPF events enhanced CCN concentrations, but in other cases no increase of CCN concentrations could be seen.

THU34

16:00-16:15

In-situ aerosol nanoparticle characterization by small angle x-ray scattering (SAXS)

Paulus Bauer (1)

Heinz Amenitsch (2), Paul M. Winkler (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Institute of Inorganic Chemistry, Graz, AUT

A main task in aerosol science is the measurement of airborne particles. Especially the analysis of nanoparticles in the range between 1nm to

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50nm requires particular attention, since they cannot be observed with visible light anymore. To determine the size and number concentration of aerosol nanoparticles Differential Mobility Particle Sizer (DMPS) and Condensation Particle Counter (CPC) are mostly used. A common drawback of these techniques is that they extract the aerosol particles from their original environment. Thereby, nanoparticles can get modified or get lost e.g. by wall collisions inside the instrument, which can affect the measured size distribution and concentration (Wang, J. et al. (2002). J. Aerosol Sci. 33, 6, 843). Hence, an in-situ measurement technique can overcome these shortcomings of conventional aerosol instruments. Small-angle X-ray scattering (SAXS) is capable to measure in-situ particle size distribution in the nanometer range.

Here we report experiments on nanoparticle characterization by SAXS conducted at the Elettra synchrotron near Trieste, Italy. The Austrian SAXS beamline was chosen due to the available high beam intensity and the experience on aerosol studies in flow tubes (Jungnickl et al. (2011), Aerosol Sci. Technol., 45, 805). To provide a representative environment for aerosols a flow tube was operated at ambient pressure with a particle concentrations of about 10^6 /cc. We analyzed high molecular weight tungsten oxide particles having a high scattering contrast compared to the air background. Conventional aerosol measurements like a Differential Mobility Particle Sizer (DMPS) and a Condensation Particle Counter (CPC) were run in parallel for direct comparison to the SAXS data. Results show that SAXS can be used to obtain in-situ size information of nanoparticles at close-to-ambient concentrations.

THU35

16:15-16:30

Modelling the dynamics of language competition in Carinthia, Austria

Katharina Prochazka

Gero Vogl

Faculty of Physics, University of Vienna, Vienna, AUT

Languages, like atoms in a solid, are constantly in motion. Through this movement, languages can spread, i.e. the region where they are used becomes larger. Oftentimes, the spread of one language means that

another language is replaced and ultimately, languages may even die out. To try to predict these developments and develop intervention measures, computer simulations and mathematical models are used. These models apply the concept of physical diffusion (movement of atoms) to linguistics (movement of languages) and allow the tracking of language spread over time and space.

We present a spatio-temporal model to simulate the spread of language in Carinthia, Austria where use of the minority language Slovenian has been steadily declining while use of the dominant language German increases. In our microscale model, the surveyed geographic area is divided into lattice cells. For each cell and time-step, the probability p of speaking a language is proportional to the number of speakers present in the preceding time step as well as to the interaction with other speakers of the same language. The model is calibrated using empirical data from the Austrian census (1880-2001), allowing us to follow the evolution of language use in Carinthia over time and space for which we present results.

Additionally, we compare the results from our microscale model with a basic reaction-diffusion model for the same system. In reaction-diffusion models, the fraction of people in the population speaking a language is described by differential equations based on Fick's laws of diffusion. This approach lets us view language spread on a macro-scale where languages are viewed as waves advancing through the country. However, treatment of language spread by reaction-diffusion equations breaks down when a continuous language area no longer exists and the language is only present in non-connected scattered islands. Such a situation of isolated language islands as in Southern Carinthia after World War II can however be described by our micro-simulation which is able to track local changes and thus offers an advantage over treatment by reaction-diffusion equations.

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Open Discussion

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THU36

13:45-14:00**Crystalline growth of ice - Restructuring of the first wetting layer during multilayer formation observed by scanning tunneling microscopy**Barbara A. J. Lechner*Technische Universität München, Garching, GER*

The growth of water layers on single crystal surfaces has been studied intensively, yet many questions still remain [1]. Comprehensive studies revealed a surprisingly complex structure in the first wetting layer, showing that the strain caused by the mismatch of the hexagonal planes in the ice crystal structure and the lattice of the substrate is released by the formation of rotated hexagons, pentagons and heptagons of molecules in addition to strongly bound hexagonal rings commensurate with the substrate [2,3]. A range of experimental and theoretical investigations showed that, on many substrates, the water monolayer does not expose any dangling hydrogen bonds as all water molecules adsorb either flat-lying or with a hydrogen atom pointing towards the surface [1,4]. Growth of multilayer water films that preserve the “down-pointing” average dipole orientation of water has been proposed to occur in some cases, resulting in the formation of “ferroelectric ice” [5]. However, the growth of the entropically more favorable proton-disordered ice requires flipping some of the molecules in the first layer to expose dangling hydrogen bonds. Such molecular reorientation may be kinetically hindered, and has been invoked to be the reason for the hydrophobic character of many water monolayer films at low temperatures [4]. Here, we present high-resolution scanning tunneling microscopy (STM) measurements of water layers adsorbed on Pt (111) and Ru (0001) to study the transition from the first layer to multilayers [6]. We observed that a second water layer initially grows in an amorphous structure

when grown on the crystalline monolayer containing pentagons, hexagons and heptagons of water molecules. To facilitate the growth of ice in a bulk-like hexagonal arrangement, the first wetting layer needs to rearrange into a hexagonal structure commensurate with the surface. Complementary STM measurements confirmed the facile re-orientation of certain molecules in the water monolayer on Pt (111) upon adsorption of ammonia (NH_3) molecules [7]. We found that NH_3 binds preferentially to H_2O molecules that are slightly elevated from the surface and weakly bound to the metal. Density functional theory (DFT) calculations showed that as the NH_3 molecule descends onto the water adlayer a high-lying water molecule reorients with zero energy barrier to expose a dangling OH ligand to H-bond NH_3 . Ammonia molecules thus detect locations in the wetting layer where a water molecule can change its orientation relatively easily to flip up a hydrogen atom.

- [1] Hodgson, A.; Haq, S. *Surf. Sci. Rep.* 2009, 64, 381–451.
- [2] Tatarkhanov, M.; Ogletree, D. F.; Rose, F.; Mitsui, T.; Fomin, E.; Maier, S.; Rose, M.; Cerdá, J. I. *J. Am. Chem. Soc.* 2009, 131, 18425–18434.
- [3] Nie, S.; Feibelman, P. J.; Bartelt, N. C.; Thürmer, K. *Phys. Rev. Lett.* 2010, 105, 026102.
- [4] Kimmel, G. A.; Petrik, N. G.; Dohnálek, Z.; Kay, B. D.; Kimmel, G. A.; Petrik, N. G.; Dohnálek, Z.; Kay, B. D. *J. Chem. Phys.* 2007, 126, 114702.
- [5] Su, X.; Lianos, L.; Shen, Y. R.; Somorjai, G. A. *Phys. Rev. Lett.*, 1998, 80, 1533–1536.
- [6] Maier, S.; Lechner, B. A. J.; Somorjai, G. A.; Salmeron, M. J. *Am. Chem. Soc.*, 2016, 138, 3145–3151.
- [7] Lechner, B. A. J.; Kim, Y.; Feibelman, P. J.; Henkelman, G.; Kang, H.; Salmeron, M. J. *Phys. Chem. C*, 2015, 119, 23052–23058.

THU37

14:00-14:15**Combined Experimental and Computational Study of Water on Fe₃O₄ (001)**Jan Hulva (1)

Matthias Meier (2), Jirí Pavelec (1), Sebastian Maaß (1), Roland Bliem (1), Michael Schmid (1), Ulrike Diebold (1), Cesare Franchini (2), Gareth Parkinson (1)

(1) Institut für Angewandte Physik, TU Wien, Wien, AUT (2) Faculty of Physics, University of Vienna, Vienna, AUT

The interaction of water with metal-oxide surfaces is an important topic for a wide range of technological and environmental applications. This is particularly true for the iron oxides because of their abundance in nature and their use in chemical processes where water is involved e.g. the water-gas shift reaction [1]. Recent studies of water on iron oxide surfaces have found significant complexity, with evidence for pressure dependent adsorption, mixed-mode adsorption and coverage dependent hydrogen bonding [2-4]. Here we use a multi-technique experimental approach combined with ab-initio calculations including molecular dynamics to disentangle the coverage and temperature dependent behavior of water on the reconstructed Fe₃O₄ (001) - ($\sqrt{2}\times\sqrt{2}$) R45° surface [5].

Temperature programmed desorption shows that the first monolayer of water desorbs from the surface in four distinct peaks between 150 K and 250 K. Based on XPS, STM images and ab-initio calculations, we conclude that the first three peaks originate from molecular water desorbing from a coverage-dependent hydrogen-bonded network, while the last peak results from recombinative desorption from a partially dissociated water trimer species. Two additional desorption states at 340 K and 520 K are ascribed to desorption from surface defects and recombinative desorption of the surface surface hydroxyl groups, respectively.

[1] Parkinson, G.S., "Iron oxide surfaces", Surface Science Reports (2016)

[2] Dementyev, P., et al. "Water Interaction with Iron Oxides." Angew. Chem. Int. Ed. 54 (2015): 13942

[3] Mulakaluri, N., et al. "Partial dissociation of water on Fe₃O₄ (001): Adsorbate induced charge and orbital order." Phys. Rev. Lett. 103 (2009): 176102.

[4] Kendelewicz, T., et al. "X-ray photoemission and density functional theory study of the interaction of water vapor with the Fe₃O₄ (001) surface at near-ambient conditions." J. Phys. ChemC 117 (2013): 2719-2733.

[5] Bliem, R., et al. "Subsurface cation vacancy stabilization of the magnetite (001) surface." Science 346 (2014): 1215-1218.

THU38

14:15-14:30

Water Adsorption on Magnetite: Insights from DFT

Matthias Meier (1)

Jan Hulva (2), Jiri Pavelec (2), Sebastian Maaß (2), Roland Bliem (2), Michael Schmid (2), Ulrike Diebold (2), Cesare Franchini (1), Gareth S. Parkinson (2)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Institute of Applied Physics, Vienna University of Technology, Vienna, AUT

Metal oxides are used in a wide range of applications and chemical processes such as the water-gas shift reaction [1]. The interaction of their surfaces with water - which is involved in the reaction - is therefore an important topic. Recent studies of water on these surfaces have found significant complexity, with evidence for mixed-mode adsorption and coverage dependent hydrogen bonding [2]. A combination of experimental techniques and density functional theory (DFT) calculations is used in order to study the adsorption of water on the Fe₃O₄ (001) surface, on the previously determined SVC structural model [3]. Temperature programmed desorption (TPD) shows 4 distinct peaks between 150 K and 250 K corresponding to the desorption of the first monolayer of water, consisting of 9 molecules. Calculations indicate 9 adsorption sites with coverage-dependent adsorption energies which can be explained by the existence of a hydrogen bonded network. Molecular dynamics (MD) simulations are used to determine the most stable configurations of n molecules (with $9 \leq n \leq 0$). Energy minimization (at 0 K) of these configurations allow to draw the surface phase diagram as

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a function of the water chemical potential. Nudged elastic band (NEB) calculations give access to activation energies required during the re-organization of water molecules, which is observed by MD (in-between 2 successive desorptions). keywords: Magnetite, Fe₃O₄, TPD, DFT, MD, NEB, hydrogen bond

[1] G. S. Parkinson, Surf. Sci. Rep. (2016).

[2] N. Mulakaluri, R. Pentcheva, and M. Scheffler, J. Phys. Chem. C 114, 11148 (2010).

[3] R. Bliem et al., Science 346, 1215 (2014).

THU39

14:30-14:45

Adsorption and stability of Catechol on Iron Oxide Thin Films: A comparing UHV-liquid study

Sascha Pomp

P. Seidel, M. Hollerer, M. Sterrer

University of Graz, Graz, AUT

As a building block of many environmentally and industrially important chemicals, Catechol is used in photographic development, pharmaceuticals and as a dye. In many of these systems the interaction of catechol with an oxide substrate plays a key role. Here, we focused on the investigation of Catechol adsorption and stability on well-known surfaces as bare Pt (111), FeO/Pt (111) and Fe₃O₄/Pt (111) in a temperature range of 100 K to 600 K in UHV, subsequently transferring this knowledge to ambient conditions and liquid phase. Concentrated attention was attracted by the FeO film with its additional possibility to form a hydroxyl terminated trilayer with a (Pt-) O-Fe-OH stacking, which was thought to act as an anchoring site, especially for the hydroxyls groups of Catechol. Therefore, we present classical surface science methods as X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), low-temperature scanning tunneling microscopy (LT-STM) and low-energy electron diffraction (LEED) combined with characterization of the deposition of the molecule from aqueous phase, which is characterized by cyclic voltammetry (CV) in combination with the previously mentioned UHV methods.

THU40

14:45-15:00

Fluoride-free wet-chemical preparation of oxide single crystal surfaces

Stijn F. L. Mertens

Matthias Müllner, Jan Balajka, Michael Schmid, Ulrike Diebold

Institut für Angewandte Physik, TU Wien, Vienna, AUT

The ultimate goal to perform surface science studies under technologically relevant conditions includes wet-chemical methods to prepare well-defined oxide surfaces [1]. The most widely practised approach is hydrofluoric acid etching, even though this chemical poses serious health risks and may inadvertently dope the surface with fluorine, an efficient electron donor [2].

Here, we present a rational yet versatile wet-chemical alternative to lengthy sputtering-annealing cycles in ultrahigh vacuum for preparing single crystal oxide samples for surface science investigations. The method does not require hydrofluoric acid, is environmentally benign and is demonstrated on rutile TiO₂ (110), rutile TiO₂ (011) and SrTiO₃ (100), but may have much wider application potential, also for surfaces that are quickly destroyed by acids.

The procedure consists of (i) ultrasonication in the presence of a dispersing agent to remove polishing debris; (ii) thermal annealing to produce equilibrium-shaped steps and terraces determined by the crystal miscut; and (iii) oxidative cleaning in an alkaline mixture to remove adsorbed organic contaminants from the surface. Each of the steps is optimised based on AFM and characterisation in ultrahigh vacuum, including by LEED and XPS. Following this wet-chemical preparation, we demonstrate atomically resolved electrochemical scanning tunnelling microscopy on TiO₂ (110), on a sample that was never treated by sputtering-annealing.

1. Ahmed, M.H.M., et al., Wet chemically prepared rutile TiO₂ (110) and TiO₂ (011): Substrate preparation for surface studies under non-UHV conditions. *Surface Science*, 2014. 630: p. 41-45.
2. Chambers, S.A., et al., Unintentional F doping of SrTiO₃ (001) etched in HF acid-structure and electronic properties. *Surface Science*, 2012. 606: p. 554-558.

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THU41

15:00-15:15

Grain boundaries and layer stacking in chemical vapour deposited hexagonal boron nitride

Bernhard Bayer (1)

Sabina Caneva (2), Timothy Pennycook (1), Jani Kotakoski (1), Clemens Mangler (1), Stephan Hofmann (2), Jannik Meyer (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) University of Cambridge, Cambridge, GBR

Hexagonal boron nitride (h-BN) is a two-dimensional (2D) insulator that is isostructural to graphene and considered as the ultimately thin dielectric layer of choice in 2D electronics. A key technological challenge is the scalable manufacture of h-BN, in particular as a continuous film of controlled layer number, crystalline quality and microstructure. Catalytic chemical vapour deposition (CVD) has emerged as the most viable technique to address this, and we have recently reported substantial improvements in obtainable control over CVD h-BN properties based on rational catalyst engineering [1,2,3].

Here, we show, via atomically-resolved scanning transmission electron microscopy (STEM) combined with bright-field and dark-field transmission electron microscopy (TEM) techniques, how to engineer a controlled grain boundary structure of self-sealing overlapping grain boundaries in h-BN layers by CVD. Combined with fundamental insights into partial non-equilibrium layer stacking in CVD h-BN layers we thus provide a framework on how to control grain boundary structure and layer stacking based on catalyst choice and processing parameters in h-BN CVD.

[1] Chem. Mater., 26, 6380 (2014),

[2] Nano Lett., 15, 1867 (2015),

[3] Nano Lett., 16, 1250 (2016). B.C.B. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 656214 - 2DInterFOX.

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THU42

15:45-16:00

Adsorption Properties of Hydrogen on Antimony (111) Probed by Helium Atom Scattering

Adrian Ruckhofer

Institute of Experimental Physics, TU Graz Graz, AUT

While antimony (Sb) is a topological semimetal, Sb nanofilms have been proposed to be topological insulators[1,2] and recent calculations showed that the adsorption of hydrogen on Sb thin films is capable of modulating the topological surface states[3,4]. The adsorption of hydrogen on metal surfaces has been the subject of many experimental and theoretical efforts in the last decades, but very little experimental data exists for the adsorption properties of semimetal surfaces apart from graphene[5,6]. We have carried out a series of helium atom scattering (HAS) measurements in order to characterise the adsorption properties of hydrogen on Sb (111). HAS is particularly useful for the investigation of adsorbed hydrogen atoms due to the much higher scattering cross section compared to electron scattering. Molecular hydrogen does not adsorb at temperatures above 110 K in contrast to pre-dissociated atomic hydrogen. Depending on the substrate temperature, two different adlayer phases of atomic hydrogen on Sb (111) occur. At low substrate temperatures (110 K), the deposited hydrogen layer does not show any ordering while we observe a perfectly ordered (1x1) H/Sb (111) structure for deposition at room temperature. Furthermore, the amorphous hydrogen layer deposited at low temperature forms an ordered overlayer upon heating the crystal to room temperature. The resulting diffraction peak intensities indicate a somewhat lower electronic corrugation of the hydrogen adlayer than of the clean Sb (111) substrate. Hydrogen starts to desorb at 430 K which corresponds to a desorption energy of (1.33 ± 0.06) eV. Using measurements of the helium reflectivity during hydrogen exposure at different surface temperatures, we conclude that the initial sticking coefficient of atomic hydrogen on Sb (111) decreases with increasing surface temperature. Furthermore, the scattering cross section for the diffuse scattering of helium from hydrogen on Sb (111) is determined as $(12 \pm 1) \text{ \AA}^2$.

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- [1] P. Kraus et al. EPL, accepted (2016).
- [2] P.F. Zhang et al. Phys. Rev. B, 85, 201410 (2012).
- [3] Bian et al. Phys. Rev. Lett., 108, 176401 (2012).
- [4] D. Wang et al. Phys. Chem. Chem. Phys., 17, 3577 (2015).
- [5] J. Shan et al. Chem. Phys. Lett., 517, 46 (2011).
- [6] C. Lin et al. Nano Lett., 15, 903 (2015).

THU43**16:00-16:15****Electron-Phonon Coupling and Atom-Surface Interaction of the Topological Insulator Bi_2Te_3 (111)**Anton Tamtög*Institute of Experimental Physics, TU Graz Graz, AUT*

We have studied the topological insulator Bi_2Te_3 (111) by means of helium atom scattering. By employing a recently developed quantum-theoretical derivation of the helium scattering probabilities[1], the electron-phonon coupling λ of Bi_2Te_3 (111) is determined. Based on the Debye-Waller attenuation of the elastic diffraction peaks of Bi_2Te_3 (111), we find a λ of 0.05. This method allows to extract a correctly averaged λ and to address the discrepancy between previous studies[2-4]. The relatively modest value of λ is not surprising even though some individual phonons may provide a larger electron-phonon interaction. Moreover, we are able to obtain an accurate He- Bi_2Te_3 (111) atom-surface interaction profile. Diffraction experiments from in-situ cleaved single crystals of Bi_2Te_3 (111) show a multitude of distinct resonance features which are used to identify the bound state energies of the interaction potential. A full three-dimensional interaction profile can be fitted to an azimuthal scan using an extended close-coupling (CC) calculation. Modelling the scattering intensities via an elastic CC calculation provides a quantum mechanically accurate way of testing a provided interaction profile against measured data[5,6].

- [1] J. R. Manson et al., Phys. Chem. Lett. 7, 1016 (2016).
- [2] C. Howard et al., Phys. Rev. B 88, 035402 (2013).
- [3] C. Chen et al., Sci. Rep. 3, 2411 (2013).
- [4] T. Kondo et al., Phys. Rev. Lett. 110, 217601 (2013).

- [5] A. S. Sanz et al., Phys. Rep. 451, 37 (2007).
 [6] P. Kraus et al., J. Phys. Chem. C 119, 17235 (2015).

THU44

16:15-16:30

Ion-beam-induced magnetic and structural phase transformation of fcc Fe thin films on different substrates

Jonas Gloss (1)

Michal Horký (2), Bernhard Ruch (1), Lukas Flajsman (2), Viola Krizakova (2), Michael Schmid (1), Michal Urbánek (2), Peter Varga (1)

(1) TU Wien, Vienna, AUT (2) Brno University of Technology, Brno, CZE

There are different approaches to ion-beam-induced magnetic patterning, for example modification of magnetic anisotropies [1], coercivity, exchange bias or the magnetization of the material. However, these approaches often lead to ferromagnetic structures embedded in a ferromagnetic (or antiferromagnetic) matrix [2]. Ultrathin Fe films on Cu (100) have been studied extensively in the past for their metastability, i.e. magnetic (paramagnetic to ferromagnetic) and structural (fcc to bcc) phase transformation upon ion beam irradiation [3, 4]. Replacing Fe by Fe₇₈Ni₂₂ removes the 4-nm thickness limit of fcc Fe films and allows for growing metastable fcc films up to 25 nm [5]. We present two new alternative substrates, which are more appropriate for applications and optical analysis techniques than the Cu (100) single crystals used so far. The first one is hydrogen terminated Si (100) with a Cu buffer layer. Cu on the H-Si (100) grows epitaxially, although not layer-by-layer [6]. Nevertheless, the growth of Fe₇₈Ni₂₂ metastable thin films is possible. The second investigated substrate is diamond C (001). It has a similar lattice mismatch to fcc Fe as Cu and the epitaxial growth of fcc Fe films with a limit of 4 ML has already been described [7, 8]. We present a thorough study of this system and its extension to Fe₇₈Ni₂₂ films. We used a 10–30 keV Ga⁺ focused ion beam (FIB) for writing the magnetic nanopatterns in the metastable films on Cu (100), Si (100) with a Cu buffer layer and C (100). The patterns were consequently studied by high-resolution Kerr magnetometry, scanning electron microscopy and magnetic force microscopy.

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- [1] C. Chappert, et al., Science 280 (5371), 1919-1922 (1998).
- [2] R. Bali, et al., Nano Lett. 14, 435-441 (2014).
- [3] C. Chappert, et al., Nature Mat. 6, 813-823 (2007).
- [3] W. Rupp, et al., Appl. Phys. Lett. 93, 063102 (2008).
- [4] S. Shah Zaman, et al. J. Appl. Phys. 110, 024309 (2011).
- [5] J. Gloss, et al., Appl. Phys. Lett. 103, 262405 (2013).
- [6] C.A.Chang, et al., Appl. Phys. Lett. 57, 2239 (1990).
- [7] D. P. Pappas, et al., Appl. Phys. Lett. 64, 28 (1994).
- [8] D. Li, et al., Phys. Rev. B 57, 16 (1998).

THU45

16:30-16:45

Temperature stability measurement of mono-metallic nanowires generated in superfluid helium droplets studied by atomic resolution electron tomography

Maximilian Lasserus (1)

Martin Schnedlitz (1), Daniel Knez (2), Alexander Volk (1), Ferdinand Hofer (2), Wolfgang E. Ernst (1)

(1) Institute of Experimental Physics, TU Graz, Graz, AUT (2) Institut of Electron Microscopy and Nanoanalysis, TU Graz, Graz, AUT

Nanostructures elongated in one dimension, such as wires, have drawn tremendous interest because of their potential application in catalysis, optics and magnetic industries. Helium nanodroplets provide an ideal matrix for aggregation of tailored nanowires. We utilize superfluid helium nanodroplets to grow different lengths of mono-metallic nanowires. Using high resolution electron microscopy we can clarify the structure and the composition and observe the temperature dependent breakup of Au, Ag, Ni and Cu nanowires at different sizes. Compared to previous measurements, we have now been able to observe the specimen in situ while raising the temperature of the substrate from 300 to 850 Kelvin. The detailed analysis shines light on the behaviour of the heated nanostructures and allows a comparison between the nanoscale properties of different metals.

THU46

16:45-17:00

Molecular dynamics simulations of experimentally observed diffusion processes on the surface of metallic nanowires

Martin Schnedlitz (1)

Andreas Hauser (1), Maximilian Lasserus (1), Daniel Knez (2), Alexander Volk (1), Ferdinand Hofer (2), Wolfgang E. Ernst (1)

(1) Institute of Experimental Physics, TU Graz, Graz, AUT (2) Institut of Electron Microscopy and Nanoanalysis, TU Graz, Graz, AUT

Metal nanoparticles, in particular metal nanowires, have experienced a tremendous growth of interest in recent years due to their application in fields such as nanoelectronics, catalysis, optics and magnetic industries. In this context, superfluid He nanodroplets provide a novel, minimally invasive tool for the creation of mono-metallic nanowires. We have studied the growth process and the temperature dependent stability of Au, Ag, Ni, Cu nanowires via atomic resolution electron tomography [1], and compared the obtained results to molecular dynamics simulations describing time- and temperature dependent surface diffusion processes. This detailed study gives first insights of the temperature accelerated self-diffusion and multicentre agglomeration of mono-metallic nanowires as a function of their initial size and composition.

[1] Georg Haberfehlner, Philipp Thaler, Daniel Knez, Alexander Volk, Ferdinand Hofer, Wolfgang E. Ernst, Gerald Kothleitner, „Formation of bimetallic clusters in superfluid helium nanodroplets analysed by atomic resolution electron tomography“, Nature Communications, 6, 8779-1-6 (2015) <http://www.nature.com/ncomms/2015/151028/ncomms9779/full/ncomms9779.html>

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THU47

17:00-17:15

Stability and Structure of TiO₂ surfaces in liquid water

Jan Balajka

Martin Setvín, Martin Calkovský, Matthias Müllner, Zdenek Jakub, Michael Schmid, Stijn Mertens, Ulrike Diebold

TU Wien, Vienna, AUT

Titanium dioxide (TiO₂) and other metal oxides offer wide range of properties that can be utilized in many industrial applications such as photocatalysis, dye-sensitized solar cells, etc. At present the surfaces are well understood under UHV conditions, however in most of industry-relevant applications the surfaces are immersed in liquid. Understanding the processes closer to real application conditions at atomic scale is crucial for further improvement and better efficiency. Therefore a combined study was carried out in which well-prepared and well-characterized surfaces in UHV were exposed to liquid water and consequently analyzed with UHV techniques (STM, XPS, LEIS, LEED) again. To do that we used a dedicated system that allows controlled and clean transfer of the studied sample between UHV chamber and electrochemical cell.

As the first system prototypical TiO₂ Rutile (110) surface was studied. The results show that UHV prepared surface is unchanged by contact with liquid water and still shows unreconstructed structure. These results are also in agreement with in-situ STM studies performed, where atomically resolved STM images in liquid H₂O and also in HClO₄ electrolyte show UHV-like (1x1) surface structure.

Another studied surface was the second most common facet of TiO₂ Rutile, the (011) surface. This termination exhibits (2x1) reconstruction in UHV. Based on DFT predictions the (2x1) reconstructed surface is no longer energetically favorable in liquid water environment. The experiments carried out indicate change in surface structure upon contact with liquid water. However the possibility of contaminant-induced restructuring has to be carefully excluded.

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ERWIN-SCHRÖDINGER-HÖRSAAL

THU48

13:45-14:15

The 19th century pre-global-warming pioneers: from Joseph Fourier to Svante Arrhenius

Walter Kutschera

Faculty of Physics, University of Vienna, Vienna, AUT

Global warming is a buzzword today in almost every talk about the status of our Earth system. It seems worthwhile to take a look at a few great scientists of the 19th century, who started to think about the reasons for the relatively comfortable average temperature on the surface of the Earth. During the 19th century it was merely scientific curiosity to think about the atmosphere and its influence on the temperature on Earth. In the 1820s, the French mathematician Joseph Fourier discussed for the first time a possible greenhouse effect of the atmosphere. The quintessential paper on this issue was published in 1896 by Svante Arrhenius, the Swedish chemist and Nobel Laureate of 1903, with the intriguing title „On the influence of carbonic acid in the air upon the temperature of the ground“ (http://www.rsc.org/images/Arrhenius1896_tcm18-173546.pdf).

This talk will describe the development of ideas about the atmosphere during the 19th century, which still form the basis of our understanding of global warming and climate change.

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THU49

14:15-14:45

Physics at the University Vienna and the Radium Institute between 1913 and 1950

Franz Sachslehner

Faculty of Physics, University of Vienna, Vienna, AUT

Since 1850 the University Vienna's physics had insufficient buildings, however, 1913 a magnificent and spacious physics building was opened adjacent to the new Institute of Radium Research of the Imperial Academy of Science, which was already finished in 1910. Within a few years the Radium Institute enjoyed international reputation. For example, the discovery of the cosmic rays (Hess) and the development of the radioactive tracer method (Hevesy) were honoured with Nobel prizes later. The First World War hindered the development of the Viennese physics considerably. The hopeful theorist Fritz Hasenöhl died in the war. Hans Thirring became a defender of the theory of relativity and calculated together with Josef Lense the later so-called Thirring-Lense effect in 1918. At that time, Erwin Schrödinger and Fritz Kohlrausch were concerned with radioactivity and the physics of colours in the Second Institute of Physics, whereas the somewhat stubborn and unorthodox Felix Ehrenhaft investigated electrical charge measurement and photophoresis. In 1920, when the position of Franz Exner had to be filled, a reorganisation of the physics institutes and of the teaching duties was done. Felix Ehrenhaft got a small new institute, the Third Institute of physics, which was established at the expense of Ernst Lecher's First and Gustav Jäger's Second Physical Institute and existed until 1938. Additionally, a common library was founded managed by the Institute of Theoretical Physics. The research focus in the Radium Institute changed to the beginning nuclear physics. Famous are the photographic tracks of the disintegration of light nuclei obtained by Marietta Blau. In 1938 the discrimination of pacifistic or Jewish professors and students reached a first culmination: Hans Thirring and Stefan Meyer were dismissed, Felix Ehrenhaft was mistreated by his colleagues, Georg Stetter and Gerhard Kirsch, and was forced to emigrate as well as Marietta Blau, Karl Przibram and other scientists. So only the persons suiting the National Socialist regime headed the institutes up to 1945. During the Second World War a "Vierteljahresplaninstiut für Neutronenforschung" was

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organised. It was led by Georg Stetter and provided some resources for research. After the war the University Vienna had a shortage of staff and denazification processes were done rigorously. Physicists like Thirring and Meyer were rehabilitated. Ehrenhaft and Przibram returned to Vienna and got the head of the First and Second Institute of Physics, respectively.

THU50

14:45-15:15

Globes - sundials - topographic maps: on the 250th anniversary of Peter Anich's death

Armin Denoth

University of Innsbruck, Innsbruck, AUT

Quos coluit, dimensus agros' and ,accessit stellis ornatus agrestis': these two sentences describe the work of Peter Anich (1723-1766), a Tyrolean farmer and wood-turner, who wrote history. At a really young age he developed a great interest in Mathematics and Astronomy, got orders to renovate sundials on churches and, later-on, designed and constructed sundials showing monthly lines and even day lengths. Starting 1751, at an age of 28 years, he got practical and theoretical instructions in Mathematics, land-surveying techniques, Astronomy and especially in calligraphy by Ignaz Weinhart, Professor of Mathematics and Physics at the ,Leopoldinische Universität' Innsbruck. Weinhart realized and promoted the ingenious abilities of Anich: so, after 4 years of education, Anich created terrestrial and celestial globes, designed and constructed geodetic instruments and ring-shaped sundials (Sonnenringe), and has been assigned the challenging task to create a new map of Tirol. This map, later called the ,Atlas Tyrolensis', was the most precise, astronomical-based topographic map at this time. Some of Anich's instruments and objects have been preserved and are still in good shape: vertical sundials on churches and farmhouses, geodetic and survey instruments, the two famous giant globes and several small globes, the 2 parts of the Atlas Tyrolensis and other smaller topographic maps.

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THU51

15:45-16:30**Eine Auswahl von Demonstrationsversuchen, welche auf historische Wurzeln zurückgreifen**Leopold Stadler*Vienna, AUT*

Die Probleme der „Erstentdecker“ erlebt man hautnah beim Nachstellen historischer Experimente. Z.B. trifft dies zu auf: * den Versuch von Dulong & Petit (absolute Messung der Ausdehnung von Quecksilber), * die Messung der Brechzahl von Gasen, insbes. von Luft, Versuch nach Beot, * das altbewährte „Hemmungspendel“, dessen Erfinder zwar unbekannt ist, aber dessen tradierter Fehler mit einem aufwändigen Eigenbau aufgezeigt wird, * die „Federwaage von Jolly“. Die Experimente geben den Originalaufbau wieder mit einer Auswahl von Abbildungen aus der Zeit von 1880 bis 1910. Die Genauigkeit der historischen Versuche werden mit dem Nachbau verglichen.

AMP**SMI SEMINARRAUM**

THU52

13:45-14:00**Chiral separation via two-dimensional, porous nanostructures**Samuel Fruehwirth

Andreas Hauser

Institut für Experimentalphysik, TU Graz, Graz, AUT

In a recent study [1] we suggested a new concept of chiral separation based on functionalised nanoporous sheets of graphene. A chiral molecule, permanently attached to the pore rim, acts as a gatekeeper, and only one enantiomer may pass the membrane, whereas the other

is kept outside due to differently shaped complexes formed by the gatekeeper and each enantiomer upon transition. We further investigate the underlying separation principle in greater detail and make suggestions for suitable combinations of gatekeepers and free gas molecules. Different binary complexes are tested for their applicability to the suggested technique. Several standard force fields are applied to examine their feasibility of reproducing ab-initio data. For the same purpose, we further calculate pore transmission pathways for a selection of gas molecules and a set of graphene-related pores. In a last step we explore the behaviour of the most suitable molecule-gatekeeper combinations in QM/MM simulations with the aim to estimate selectivities and transmission rates.

[1] Hauser et al., *Angew. Chem. Int. Ed.*, 2014, 53, 9957–9960

THU53

14:00-14:15

Cavity cooling of nanoparticles for ultra-high mass matter wave interferometry

James Millen

Faculty of Physics, University of Vienna, Vienna, AUT

Is there a mass limit to quantum physics? There are various theories and interpretations that try to answer this question, and perhaps the most surprising answer would be “no”. We test this by performing matter wave interferometry with nano-scale silicon particles, by which we can dramatically increase the bounds on any limit, study the role of gravity in quantum physics and look for extensions to standard quantum theory. First, we must prepare a beam of nanoparticles which is cold enough in the direction transverse to its motion to coherently illuminate a diffraction grating. The method we use is cavity cooling, whereby a high finesse optical cavity damps the motion of transiting nanoparticles. We report cooling of translational motion, and detection and control of the rotational motion of nanofabricated, silicon nanospheres and rods in high vacuum.

To perform matterwave experiments over a sensible length scale we need to work with nanoparticles that are too small for conventional

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optical cavities. We present the development of novel silicon microcavities for experiments with particles a few nanometres in size.

THU54

14:15-14:30

Beam splitters for complex biomolecules: Conceptual & experimental explorations

Christian Brand

Christian Knobloch, Stefan Kuhn, Markus Arndt

Faculty of Physics, University of Vienna, Vienna, AUT

The high sensitivity of coherently delocalized matter-waves to external perturbations like accelerations, electric fields or van der Waals forces is the basis for a number of precision measurements. The wealth of information which can be extracted from such experiments makes it desirable to exploit them also for spectroscopy of biomolecules. Matter-wave phase shifts will allow inferring the structure and dynamics even for systems which have evaded gas phase studies so far. The key ingredient in all these studies is a matter-wave beam splitter which is suitable for biomolecules. I will present a tuneable diffraction grating based on a cavity-enhanced laser beam. Depending on the power inside the resonator we expect to see a transition from a phase-grating to an absorptive grating. By using widely tuneable lasers in combination with an external frequency doubler to pump the cavity this beam splitter can become a novel tool for molecule spectroscopy. „This contribution is ment to be for session: SFB-FoQuS“

THU55

14:30-14:45

Automated Search for new quantum Experiments

Mario Krenn

Mehul Malik, Robert Fickler, Radek Lapkiewicz, Anton Zeilinger

IQOQI/University of Vienna, Vienna, AUT

Quantum mechanics predicts a number of at first sight counterintuitive phenomena. It is therefore a question whether our intuition is the best way to find new experiments. Here we report the development of the computer algorithm MELVIN [1] which is able to find new experimental implementations for the creation and manipulation of complex quantum states. And indeed, the discovered experiments extensively use unfamiliar and asymmetric techniques which are challenging to understand intuitively. The results range from the first implementation of a high-dimensional Greenberger-Horne-Zeilinger (GHZ) state, to a vast variety of experiments for asymmetrically entangled quantum states – a feature that can only exist when both the number of involved parties and dimensions is larger than 2. Additionally, new types of high-dimensional transformations are found that perform cyclic operations. MELVIN autonomously learns from solutions for simpler systems, which significantly speeds up the discovery rate of more complex experiments.

The large number of discoveries reveals a way to investigate new families of complex entangled quantum systems in the laboratory. Several of these experiments have already been successfully built in our labs [2, 3], and hopefully many more will follow. The ability to automate the design of a quantum experiment can be applied to many quantum systems and allows the physical realization of quantum states previously thought of only on paper.

[1] Mario Krenn, Mehul Malik, Robert Fickler, Radek Lapkiewicz, Anton Zeilinger, Automated Search for new Quantum Experiments, Phys. Rev. Lett.116, 090405 (2016).

[2] Mehul Malik, Manuel Erhard, Marcus Huber, Mario Krenn, Robert Fickler, Anton Zeilinger, Multi-photon entanglement in high dimensions, Nature Photonics10, 248-252 (2016).

[3] Florian Schlederer, Mario Krenn, Robert Fickler, Mehul Malik, Anton Zeilinger, Cyclic transformation of orbital angular momentum modes, New J. Phys.18, 043019 (2016).

THU56

14:45-15:00**An optical nanofiber-based interface for single molecules**Sarah M. Skoff

Hardy Schauffert, David Papencordt, Arno Rauschenbeutel

TU Wien, Vienna, AUT

In recent years, single molecules in solids have gained increased interest as building blocks for quantum networks, quantum metrology and nanosensors. For all these applications strong light-matter interactions are essential.

A versatile tool to achieve such interactions is an optical nanofiber, which is the tapered part of a commercial optical fiber that has a sub-wavelength diameter waist. This allows an appreciable amount of light to propagate outside the fiber in the form of an evanescent waist. Due to the strong transverse confinement of the light field which prevails over the entire length of the nanofiber, the interaction with emitters close to the surface can be significant.

Here we show how single terrylene molecules in a p-terphenyl matrix can be evanescently coupled to the guided modes of optical nanofibers. This presents a new platform based on solid state emitters that is used for quantum optics and can be naturally integrated into any optical fiber based quantum network.

THU57

15:00-15:15**Acetone multi-channel photofragmentation dynamics studied by time-resolved photoelectron-photoion coincidence spectroscopy**Markus Koch

Markus Bainschab, Paul Maierhofer, Bernhard Thaler, Pascal Heim, Wolfgang E. Ernst

TU Graz, Graz, AUT

The excited state dynamics of isolated acetone molecules initiated by two-photon (269 nm) excitation to high-lying Rydberg states has been investigated with time-resolved photoelectron-photoion coincidence

techniques (PEPICO). We observe three distinct pump-probe ionization channels because of different relaxation processes triggered by the excitation pulse. The high differentiability of PEPICO detection allows us to observe the fragmentation behavior and temporal evolution of each channel separately. The first channel proceeds via excited Sn Rydberg states to the unfragmented molecular ion. A second channel via the S3 state leads to fragmentation after ionization due to electronic-to-vibrational energy conversion in the neutral molecule, as evidenced by the simultaneous presence of parent and acetyl fragment PEPICO signals. The populations of these excited states undergo an exponential decay with the same (147 ± 28) fs time constant. A third, persistent pure-fragment PEPICO signal indicates the ionization of neutral, excited acetyl radicals, which are presumably formed through Norrish type I dissociation on excited state surfaces.

THU58

15:45-16:00

A quantum router for high-dimensional entanglement

Manuel Erhard

IQOQI/University of Vienna, Vienna, AUT

One of the most interesting aspects of quantum mechanics is entanglement. Entanglement plays an important role in testing fundamental physical questions as well as in modern technology. Recently, entanglement in multiple levels, or higher dimensions, has gained increasing interest because of higher information capacity and unprecedented levels of security, for example. Here we show how a high-dimensionally entangled quantum state of two photons can be split into two entangled states in a lower dimensionality structure. Experimentally, we utilise the orbital angular momentum of photons to encode the information in multiple levels. The experimental results presented here indeed show that an initially at least 10-dimensionally entangled state can be split into two at least 5-dimensionally entangled states. Thus our work demonstrates that high-dimensional entanglement shared between two parties can be distributed two three or more parties while conserving the non-classical correlations.

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THU59

16:00-16:15

A Cosmic Bell Test

Johannes Handsteiner

IQOQI/University of Vienna, Vienna, AUT

Experimental violations of Bell inequalities in general are vulnerable to so-called “loopholes”. The major loopholes are related to locality, fair-sampling of inefficient detectors and freedom-of-choice (i.e. measurement setting independence). Compared to the locality and fair-sampling loopholes, freedom-of-choice has received far less attention, though recent calculations have demonstrated that the predictions of quantum mechanics could be reproduced by local realistic models even if the measurement settings are only a little correlated to some local hidden variables. A recently proposed “cosmic Bell” experiment suggests using light from causally disconnected cosmic sources to set the measurements. If violations of Bell’s inequality are still observed (with all other loopholes closed), a local realist explanation would require that the correlations for the measurement settings were put in place billions of years ago. As a first experiment in this direction, we have conducted a Bell test using nearby stars as bright cosmic light sources. This shifts back the time at which correlations between the measurement settings could have been established to approximately 3000 years before the experiment. The long-term goal is to “replace” nearby stars with the most distant quasars which are not causally connected since the earliest stages of the universe. From an experimental point of view, quasars however are significantly fainter than stars and thus require large telescopes to collect their light in order to ensure the feasibility of the experiment.

This experiment has been supported by grants of the Austrian Science Foundation (FWF) under project SFB F4008, the Austrian Research Promotion Agency (FFG) and by the Federal Ministry of Science and Research (BMWF).

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THU60

16:15-16:30

[SFB-FoQuS] Spectrally resolved measurements with semiconductor waveguides for photon pair emission

Benedikt Pressl (1)

Kaisa Laiho (1), Thomas Günthner (1), Alexander Schlager (1), Holger Suchoamel (2), Jonas Geßler (2), Martin Kamp (2), Sven Höfling (2), Christian Schneider (2), Gregor Weihs (1)

(1) Institut für Experimentalphysik, Universität Innsbruck, Innsbruck, AUT (2) Technische Physik, Universität Würzburg, Würzburg, GER

The process of parametric-down-conversion (PDC) is widely used to create photon pairs. Usually, this is carried out with bulky nonlinear crystals. Instead, here we use so called Bragg-reflection waveguides (BRWs) which are ridge waveguides etched from multi-layer aluminum gallium arsenide [1]. Switching to semiconductor materials gives access to mature fabrication techniques and allows potential integration with light sources, electronics and detectors. Investigating and evaluating their performance is crucial for future applications. As the BRWs are intrinsically multimode, only certain higher-order, spatial modes are matched for PDC interaction. The PDC process parameters that define the joint spectrum of the photon pairs depend on the classical, linear optical parameters of the modes of the waveguide, like refractive index and group refractive index. In terms of general performance, the loss coefficient, the facet reflectivity and relative mode excitation are also of interest. Experimentally, however, these parameters may be difficult and cumbersome to measure. Often, indirect methods have to be used. In this work we present a series of simple, linear and nonlinear optical experiments which allow the direct determination of these parameters. First, we record the linear transmission spectrum at both the near-infrared and telecom range. This results in Fabry-Perot fringes due to the high refractive index contrast between the waveguide and the surrounding air. The fringes are investigated with Fourier analysis which yields reliable, modally-resolved values for the group index, loss and relative excitation [2]. Then, the spectra of the emitted PDC photons are analysed to estimate the group index dispersion and the PDC phase-matching [3]. Experimentally obtained values for these parameters are much more accurate than simulations, which are limited by

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uncertainties in the refractive index models used and differences due to fabrication tolerances. Having actual, accurate values enables us to better understand current samples and improve the design of future ones.

[1] R. Horn et al, "Monolithic source of photon pairs". Phys. Rev. Lett. 108, 153605 (2012).

[2] B. Pressl et al, "Mode-resolved Fabry-Perot experiment in low-loss Bragg-reflection waveguides". Opt. Express, 23, 33608 (2015).

[3] K. Laiho et al, "Uncovering dispersion properties in semiconductor waveguides to study photon-pair generation", arxiv:1605.00517 (2016).

THU61

16:30-16:45

Classical and quantum properties of wave packet dynamics

Natascha Riahi

Faculty of Physics, University of Vienna, Vienna, AUT

We present a new method to derive exact and intuitive solutions of the time-dependent Schrödinger equation without identifying the possible eigenvalues. We analyze this solution for the special case of the asymmetric square well (a box with exit) and we discuss the classical and quantum aspects of the wave packet behaviour within the semiclassical time range. We can also show that the form of the solution we have found for the box with exit is a combination of the solutions of the infinite square well and the potential step.

THU62

16:45-17:00

Creation of RbCs Feshbach molecules in an optical lattice with high filling fraction

Silva Mezinska

University of Innsbruck, Innsbruck, AUT

Ultracold dipolar systems are of high interest for quantum chemistry, precision spectroscopy, quantum many-body physics, and quantum simulation. The goal of our project is to prepare an ultracold sample of dipolar RbCs ground-state molecules in an optical lattice with a high filling factor. To this end, atomic Rb and Cs samples are mixed in an optical lattice to efficiently form Rb-Cs atom pairs as precursors to ground-state molecules. The basic idea is to go through the superfluid-to-Mott-insulator phase transition twice, first for Cs to create a sample with single-site occupancy, then for Rb on top of Cs to create a homogenous distribution of atom pairs.

We investigate the transport properties of superfluid Rb samples while they are moved on top of a strongly interacting sample of Cs atoms. Overlapping is realized in the vicinity of a Feshbach-resonance zero crossing to tune the interspecies interactions. Our experiments show that atom-pair formation is optimized for nulled interactions. We estimate the filling fraction to be 30% in the center of our trap.

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in front of Josef-Stefan-Hörsaal**

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PT01

Structural arrangement of methyl ammonium molecules in lead iodine perovskites

Jonathan Lahnsteiner

Menno Bokdam, Georg Kresse

Faculty of Physics, University of Vienna, Vienna, AUT

In the last 3 years the performance of perovskite solar cells has increased spectacularly, from 10% to 20% solar cell efficiency. We investigate the methyl ammonium lead iodide (MAPbI₃) perovskite system. It is composed of an inorganic lead iodide framework with the methyl ammonium molecules locked within Pb-I cages.

Ab-initio molecular dynamic simulations have been carried out at different conditions to determine several important properties of the organo halide perovskite system. Within this work we were able to determine a well defined ordering pattern of the organic molecules relative to each other within the perovskite system. At low temperature

the relative angles of a molecule to its neighbours in the first, third and fifth coordination sphere are approximately 180° and 60°. The second, fourth and sixth coordination spheres prefer orientations to the considered organic molecule of about 0° or 120°. The organic molecules show this ordering behaviour throughout the entire supercell. Here we used a 6x6x6 super cell, with a volume $\sim 38^3 \text{ \AA}^3$. We show that there exist orientations for the organic molecules in the organo halide perovskite systems which are clearly avoided and others which are favoured. The structural properties were considered under different simulation conditions. One parameter which is adjustable is the temperature. The temperature dependent dynamical behaviour of the organic molecules leads to several competing phases within the super cells at higher temperatures.

The influence of the crystal phase (orthorhombic, tetragonal, cubic) on the dynamics of the molecules was studied. These simulations indicate that the before mentioned ordering patterns of the methyl ammonium molecules are strongly influenced or determined by the so chosen symmetry of the inorganic lead iodide framework.

PT02

Structural and elemental analysis of individual nanocrystals embedded in an amorphous matrix by transmission electron microscopy

Stefan Noisternig (1)

Christian Ebner (1), Christoph Gammer (2), Christian Rentenberger (1), Christian Gspan (3), Hans-Peter Karnthaler (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, AUT (3) FELMI-ZFE, TU Graz, Graz, AUT

Nano-sized crystals in an amorphous matrix are considered to change the mechanical properties of an amorphous alloy. In many cases, nanocrystals are formed by special heat treatments. Here, we show that nanocrystals can emerge out of the amorphous phase during severe plastic deformation. This can be revealed by studying the composition and the atomic structure of the crystals using different transmission electron microscopy (TEM) methods.

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Disc shaped samples of a $L1_2$ long range ordered Co_3Ti alloy were deformed by high pressure torsion (HPT) using a pressure of 4 GPa and 80 rotations of one anvil. Regions of severely deformed crystalline material and regions of amorphous material revealing both the same chemical composition are recognized by scanning electron microscopy in the as-deformed samples.

A TEM analysis shows that nanocrystals of about 5 nm to 20 nm in diameter are distributed homogeneously mainly inside band shaped amorphous regions. The shape of the nanocrystals is roughly spherical and they reveal a volume fraction of $< 3\%$. The embedded nanocrystals occur in TEM specimens that are prepared by electrolytic polishing or by mechanical polishing followed by ion milling. Thus, the nanocrystals are not artifacts of the TEM specimen preparation, but they are formed during the severe plastic deformation process.

The chemical composition of nanocrystals and surrounding amorphous matrix is studied by electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope. Broad plasmon peaks with weak maxima are present in electron low energy loss spectra. Here a procedure is developed to separate a zero-loss peak from the remaining electron low energy loss spectrum even for noisy spectra and broad plasmon peaks. Based on this separation the specimen thickness can be calculated and the effect of plural inelastic scattering in electron high energy loss spectra can be compensated. Nanocrystals are surrounded by the amorphous matrix also in the direction of the incident electron beam. Since the specimen thickness is known, the influence of the amorphous matrix on the derived chemical composition of embedded nanocrystals can be estimated and corrected. The resulting chemical compositions indicate that nanocrystals of $L1_2$ long range ordered Co_3Ti , of C36 Laves phase $Co_{2.1}Ti_{0.9}$ and of C15 Laves phase Co_2Ti are formed in the amorphous matrix by polymorphous dynamic crystallization.

The presence of these structural phases is confirmed by high resolution transmission electron microscopy (HRTEM) of the embedded nanocrystals. The HRTEM analysis is supported by HRTEM simulations for the three considered phases.

A study of the edge region at the specimen hole by EELS and HRTEM reveals that a Co_3O_4 surface layer covers the TEM specimen. This layer is also nanostructured above amorphous regions and shows lattice fringe contrast in HRTEM images even at the amorphous matrix.

PT03

Low-dimensional metal-organic nanostructures

Hidetsugu Shiozawa (1)

Oleg Domanov (1), Johannes Kampfmüller (1), Georg Zechner (1), Yuta Sato (2), Kazu Suenaga (2), Takeshi Saito (2), Eugen Weschke (3), Michael Eisterer (4), Wolfgang Lang (1), Herwig Peterlik (1), Thomas Pichler (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JPN (3) Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, GER (4) Atominstitut, TU Wien, Wien, AUT

Molecular arrays and nanomagnets that are assembled in low-dimensional nanostructures can outperform their bulky counterparts. Our experiments using Raman, UV-vis-IR absorption, photoemission, SQUID, X-ray magnetic circular dichroism spectroscopy (XMCD), XRD, transmission electron microscopy (TEM), and magnetotransport measurements probe electronic and magnetic interactions at molecular interfaces that are responsible for their unique physical properties. We show that encapsulated inside single-wall carbon nanotubes (SWCNTs) or carbon fibers, ferromagnetic transition metal clusters behave as stable single-domain magnets exhibiting large coercive fields as the cluster size becomes as small as the exchange length. Metal ions in coordination compounds arranged in one dimension are ideal systems in which we study anisotropic magnetic coupling. In metal-organic frameworks (MOFs), metal ions are coordinated to form low-dimensional metal frames and porous structures. Arrays of metal ions exposed to the interior voids react with infiltrating molecules, leading to MOF's gas-sensing abilities. We demonstrate that the MOF's optical band gap, electrical conduction and magnetic ordering temperature can be tuned by molecular doping.

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PT04

In-situ X-ray scattering of spruce wood with variation of load and humidity

Alexander Müllner

Daniel Gitschthaler, Herwig Peterlik

Faculty of Physics, University of Vienna, Vienna, AUT

Due to its availability as natural resource and its good cost-efficiency, wood has become a material of increasing interest for constructing industries in recent years. A particular advantage of wood is its high strength and fracture toughness, whereas humidity could be a limiting factor because it is often accompanied by swelling, softening and fungal infestation.

To investigate structural changes at the nanoscale, we performed in-situ X-ray scattering of spruce wood by varying load and humidity. A suited X-ray transparent chamber was developed, which enables measurements at variable strains in a humidity range between 0% and 100% (0.1% precision). For the wide-angle X-ray scattering (WAXS) signal, an image plate at a sample-to-detector distance of 5.1 cm was used, whereas the small-angle X-ray scattering (SAXS) intensity passed through a hole in the WAXS imageplate and was detected by a second image plate at a distance of 65.6 cm.

From both, SAXS and WAXS intensities, the microfibril-angle and the fibril diameter were evaluated. It turned out that the laboratory X-ray intensities are not sufficient to measure a dependence on the strain as successfully reported from synchrotron experiments [1]. However, the influence of humidity could be clearly detected: An increasing fibril diameter was observed and can be explained with swelling of fibrils by absorption of water.

[1] Zabler S., Paris O., Burgert I., Fratzl P. - Moisture changes in the plant cell wall force cellulose crystallites to deform. *J. Struct. Biol.* 171 (2010) 133-141

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PT05

Freezing and thawing of aqueous solutions in emulsions

Astrid Hauptmann

University of Innsbruck, Innsbruck, AUT

The freezing behaviour of aqueous solutions in different emulsions is investigated by analytical methods such as differential scanning calorimetry and optical cryomicroscopy. We show that freezing temperature, freeze concentration and correspondingly cold-crystallization and melting change depending on the properties of the surrounding oil and emulsifier, size distribution of emulsified droplets and the parameters of emulsification. Relevance to freezing of cloud droplets is discussed.

PT06

Flash-annealed CuZr based bulk metallic glass studied by electron microscopy

Christoffer Müller (1)

Christian Ebner (1), Christoph Gammer (1), Konrad Kosiba (2), Benjamin Escher (2), Simon Pauly (2), Jürgen Eckert (3), Christian Rentenberger (1)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Institute for Complex Materials, IFW Dresden, Dresden, GER (3) Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, AUT

Bulk metallic glass (BMG) is an amorphous material with no long-range order. Still, topological and chemical short-range or medium-range order is expected to occur. The unique atomic structures of BMG lead to interesting physical and mechanical properties that make them useful for potential applications. To circumvent the limited ductility of BMG, the concept of heterogeneous microstructure by forming composites has recently been used [1]. One route to achieve a composite structure is thermal treatment of the BMG. Here we present the structure of flash-annealed CuZr based BMG.

During the flash-annealing process the structure of BMG samples is modified by heating to different target temperatures above glass

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transition temperature and subsequent rapid cooling in a water bath. $\text{Cu}_{44}\text{Zr}_{44}\text{Al}_8\text{Hf}_2\text{Co}_2$ samples were heated to temperature of 817 K, 898 K and 916 K.

Scanning electron microscopy observation of the 916 K sample reveals both an amorphous and a crystalline part with a transition area of amorphous material containing crystallites of different size in between. The diffraction pattern (DP) of a FIB lamella prepared from a single crystallite contains superlattice reflections which indicate the presence of the B2 ordered structure. It is interesting to note that in crystalline CuZr based materials, devitrified from the amorphous structure, $\text{Cu}_{10}\text{Zr}_7$ and CuZr_2 structures are expected to occur.

To obtain structural information of the samples flash-annealed to 817 K and 898 K, fluctuation electron microscopy (FEM) was applied since no indication of crystallization was found. Tilted dark field (DF) images show intensity variations in form of speckles as a result of local structural correlations. Statistical analysis of a series of DF images acquired at different scattering vectors k and angles φ yields mean intensity and normalized variance as a function of k .

Based on our results flash-annealing of CuZr based BMGs facilitates the formation of the B2 ordered crystalline structure as a metastable phase. In the amorphous phase of all samples the presence of a significant medium range order can be concluded from peaks in the normalized variance curve of DF FEM analysis. We kindly acknowledge financial support by the Austrian Science Fund (FWF): [I1309, J3397].

[1] J. Eckert, J. Das, S. Pauly, C. Duhamel, *Journal of Materials Research* 22, 285 (2007).

PT07

Dynamik von Wachstumsprozessen im Inneren von einwandigen Kohlenstoff Nanoröhrchen

Hans Kuzmany (1)

Lei Shi (1), Thomas Pichler (1), Takeshi Saito (2)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN

Kleine Moleküle können in Kohlenstoff Nanoröhrchen (KNR) eingelagert und dort chemischen Reaktionen unterworfen werden. Prozesse in diesen Nanoreaktoren sind besonders interessant, wenn es sich bei den eingelagerten Substanzen um kohlenstoffreiche Moleküle handelt. Bei diesen kommt es zur Bildung von inneren Röhrchen oder, wie wir hier zeigen, auch zu flachen Kohlenstoff Streifen (carbon nano ribbons). Das klassische Beispiel sind Befüllungen mit Fullerenen. Die Dynamik des Wachstumsprozesses der inneren Röhrchen, der Temperaturen von 1100–1200 °C erfordert, wurde analysiert. Ein ähnliches Verhalten zeigen Befüllungen mit Perylen (polyaromatischer Kohlenstoff). Im Gegensatz dazu wachsen innere Röhrchen nach Befüllung mit Metallocenen (MCp₂, M=Fe oder Pt) schon bei Temperaturen um 500 °C. Im speziellen Fall wird davon ausgegangen, dass Fe bzw. Fe₃C im Inneren des Röhrchens als Katalysator wirkt und daher die niedrige Reaktionstemperatur ermöglicht. Sind die Röhrchen sehr dünn, mit Durchmessern kleiner als 1,3 nm, so wachsen aus den Katalysatorpartikeln zusätzlich oder ausschließlich ribbonartige Kohlenstoffmoleküle. Diese Moleküle sind im Raman Spektrum nachweisbar. Sie zeigen Resonanzanregungen bei 1.85 bzw. 2.25 eV und haben Raman Linien, die für flache Kohlenstoffe typisch sind. Die Umwandlung der Metallocene in Nanoribbons erfolgt bei 500 °C schon innerhalb von Sekunden. Work supported by the Austrian Science Foundation, Project P27769-N20

PT08

Determination of the temperatures of the thermal relaxation processes in Nylon 6,6 by Raman Spectroscopy

Durval Bertoldo Menezes

Andreas Reyer, Maurizio Musso

University of Salzburg, Salzburg, AUT

When the temperature of a semi-crystalline polymer sample increases up to the melting point, some relaxation processes caused by thermally activated molecular rearrangements can happen in the form of conformational changes and microscopic deformations. Associated with these relaxation processes are variations in the thermal, mechanical and dielectric properties of the polymer sample, enabling their

detection. The relaxation range of polymeric materials is composed basically of three relaxation processes, known as α , β and γ , in order of increasing temperature, the temperature ranges where these processes happen being labeled with characteristic relaxation temperatures T_α , T_β and T_γ . The objective of this study is to show that Raman spectroscopy can be used as an additional tool to determine the temperature ranges where α , β and γ relaxation processes in polymeric materials get activated, this spectroscopic technique being sensitive to conformational changes and microscopic deformations within the polymeric structure, therefore delivering information directly from the source where these processes occur. Raman spectra of a Nylon 6/6 sample were collected in the spectral range from 100 to 3500 cm^{-1} and with spectral resolution (FWHM) of 4.0 cm^{-1} using a laser excitation wavelength of 532 nm. The polymeric sample was measured without any physical or chemical pretreatment. The temperatures of the sample inside a heating-freezing stage were set with steps of 10.0 $^\circ\text{C}$ each in the range from -120 $^\circ\text{C}$ to 120 $^\circ\text{C}$, using in between a heating rate of 20 $^\circ\text{C}$ min^{-1} . From the Raman spectrum of Nylon 6,6 obtained at -120 $^\circ\text{C}$ as reference spectrum, all the other Raman spectra at higher temperatures were subtracted in order to identify which Raman bands suffered evident changes as a function of temperature. In the case of Nylon 6,6, the peak at around 3300 cm^{-1} associated with the stretching vibration (N-H), the peak at around 1637 cm^{-1} associated with the Amide I stretching vibration (C=O), and the peak at around 1130 cm^{-1} associated with skeletal stretching vibrations (C-C) showed the most evident changes. We fitted the peaks at 3300 cm^{-1} and 1130 cm^{-1} by using a Lorentzian function and the peak at 1637 cm^{-1} by using an asymmetric Lorentzian function, obtaining the following information: FWHM, Raman peak height, integrated Raman intensity (IRI), and Raman shift. All these data were plotted as function of temperature, in order to recognize temperatures ranges which can be attributed to α , β and δ relaxation processes, enabling the determination of characteristic relaxation temperatures which are in reasonable agreement with values reported from measurements of thermal, mechanical, and dielectric properties. The authors thank the Federal Institute of the Triângulo Mineiro and all the support given by the Brazilian funding agency Capes Foundation, Ministry of Education of Brazil through the mobility program Science without Borders (grant number BEX 9462/13-9), as well as the mobility partner University of Salzburg.

PT09

Bulk Nanocrystalline Soft Magnetic Fe-Si-X Alloys Achieved Through Severe Plastic Deformation

Sheraz Khakwani (1)

Martin Kriegisch (2), Christian Rentenberger (1), Roland Grössinger (3), Michael Zehetbauer (1)

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The magnetic properties of soft magnetic materials such as Fe-Si-X alloys can be strongly improved by nanocrystallization, especially if the grain size is smaller than the magnetic moment exchange length [1, 2]. Recently the methods of Severe Plastic Deformation (SPD) have proven as a top-down technique which allows to achieve nanocrystalline materials in bulk shape [3]. The current work reports on treatises to apply High-Pressure Torsion (HPT) as the most effective SPD method, to Fe-Si-X alloys such as Fe-3wt%Si, Fe-6.5wt%Si as well as amorphous and nanocrystalline FINEMET-type alloys. Thereby the HPT technique is to be used either (i) to decrease the grain size markedly below about 50 nm (ii) to achieve similar grain sizes with a maximum homogeneous distribution out of amorphous and/or nanocrystalline alloys. Most attention is paid to apply special heat treatments which remove SPD induced internal stresses and free defects (mainly dislocations) being not part of the grain boundaries, as these defects deteriorate the magnetic properties [4]. Moreover, as SPD often produces nm-range small angle grains, the question is to be clarified whether there exists a limiting grain tilt angle to account for a beneficiary exchange coupling effect or not.

For the measurement of both the dislocation density and the grain size, special methods of X-ray Line Profile Analysis (XLPA) and Transmission Electron Microscopy (TEM) will be applied. The exchange coupling effect will be verified through Magnetic Force Microscopy (MFM).

[1] Herzer, G. (2013). Acta Materialia 61 (3): 718-734.

[2] Grössinger, R., Sato, R., et al. (2003). Advanced Engineering Materials 5 (5): 285-290.

[3] Zehetbauer M. J. and Zhu Y. T., eds. (2009). Wiley VCH Weinheim, Germany.

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[4] Zehetbauer, M. J., Grössinger R., et. al., (2010). Advanced Engineering Materials 12 (8): 692-700.

PT10

Brill Transition and Reversible Brill Transition in Nylon 6,6 by Raman Spectroscopy

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It is of the nature of semicrystalline polymers is to present several relaxations in the polymeric structure. These relaxations are associated with the mobility of the chain segments in the crystalline and amorphous regions of the polymer, which lead to changes in the physical properties due the interactions between crystalline and amorphous regions. In 1942, R.J Brill was the first to report the nature that we know today as the Brill transition (BT) in Nylon 6,6 (N66). Today we know that during the BT in N66, the triclinic crystal structure at room temperature is gradually replaced by a different triclinic structure at the Brill transition temperature (TB) ; this high-temperature crystalline form was described like a pseudohexagonal phase. The TB has been related determined by many techniques, e.g. differential scanning calorimetry and nuclear magnetic resonance between 160 and 180°C for N66. With temperature dependent Raman scattering measurements, it was possible to determine the vibrational behavior of nylon 6,6 during the Brill transition, and consequently to identify the main Raman bands associated with the Brill transition. These bands, named here Brill Raman bands, are centered at 1126 cm^{-1} and 1479 cm^{-1} at around room temperature. However, the BT happens at broad range of temperature from 120 to 180 °C, and still does not have its nature fully explained. We used the Raman spectroscopy to investigate the BT and, withal, verify its reversibility, since this technique was not employed for this purpose. We thank all the support given by the Brazilian funding agency Capes Foundation, Ministry of Education of Brazil through the mobility program Science without Borders, as well as the mobility partner University of Salzburg.

PT11

Neutron Holography: present status and possible extensions

Gerhard Krexner

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Neutron holography is a technique for investigating structural features of atomic arrangements at the nanoscale. It makes use of atomic nuclei probing their local environment by acting either as emitters or detectors of neutron waves. Particular strengths of the method include its sensitivity for light elements such as hydrogen, the possibility to distinguish different isotopes, and the large penetration depth of neutrons. A brief presentation of basic concepts underlying the technique will be followed by a review of experiments performed so far by different groups. Further, we discuss possible improvements and extensions needed to overcome currently existing drawbacks in order to establish neutron holography as a tool to be used as a routine for obtaining highly precise information on atomic positions including displacements and irregularities around the probe nuclei. Finally, some experiments and problems are listed which likely can be approached in the medium term using presently available neutron sources together with the impact to be expected from the completion of the European Spallation Source (ESS) under construction.

As a last point, we concisely discuss a possible variant of atomic resolution holography based on the application of high-energy photons. While X-ray and Mössbauer gamma-ray holography typically use photon energies around 10 keV, photons in the range of 500 keV have been successfully used in diffraction experiments for a long time and radiation generated by electron-positron annihilation (511 keV) is extensively applied in the study of various properties of condensed matter. The potential recording of holograms from such high-energy photons gives rise to various questions of interest.

[1] L. Cser, G. Krexner, and Gy. Török, EPL 54 (2001) 747

[2] L. Cser, Gy. Török, G. Krexner, I. Sharkov, PRL 89 (2002) 175504

[3] L. Cser, G. Krexner, M. Markó, I. Sharkov, Gy. Török, PRL 97 (2006) 255501

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[4] M. Markó, G. Krexner, J. Schefer, A. Szakál, L. Cser, *New J. Phys.* 12 (2010) 063036

[5] A. Szakál, M. Markó, G. Krexner, L. Cser, *EPL* 111 (2015) 26002

[6] L. Cser, G. Krexner, M. Markó, A. Szakál, in *Fundamentals of Picoscience*, Chapter 9, pp. 161-178, Ed. by Klaus D. Sattler, ISBN 13: 9781466505094, Taylor & Francis, 2013

FAKT, TUESDAY

PT12

Search for a violation of the Pauli Exclusion Principle with electrons

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The Pauli Exclusion Principle (PEP) is the foundation for our understanding of physics where systems of fermions are concerned. Therefore, it is important to make precision tests of the PEP. In a pioneering experiment, Ramberg and Snow supplied an electric current to a Cu target, and searched for PEP violating atomic transitions of the “fresh” electrons from the current. The non-existence of the anomalous X-rays from such transitions then set the upper limit for a PEP violation. The VIP (Violation of Pauli Exclusion Principle) experiment improved this method. The experiment and the results will be presented. The preliminary results of the first data taking period of the follow-up experiment VIP2 will be presented.

PT13

Silicon strip sensors made in Austria for upcoming upgrades of LHC experiments

Axel König

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The luminosity of the LHC at CERN is continuously increasing and will experience a major enhancement after the third long shutdown (LS3) scheduled around 2023. The resulting increase in pile-up and radiation damage constitutes several challenges to the tracking detectors of the LHC experiments. Moreover, the lifetime of these detectors is limited due to accumulated radiation damage and will reach its end until LS3. These issues demand for upgrades of the tracking detectors involving several hundreds of square meters of silicon strip sensors. Recent developments as well as results on the evaluation of silicon strip sensors produced in Austria are presented where the development aims for the demanded large scale production. The sensors exhibit n-on-p technology, are AC-coupled and processed on 8-inch wafers. They represent the world's first AC-coupled silicon strip sensors produced on 8-inch wafers. Results of the electrical characterization as well as investigations concerning strip isolation are presented. In particular, different implantation variations were tested at the manufacturer and analyzed in the laboratory. Conventional as well as new types of test structures were measured giving insights into the process quality and revealing possible optimizations for future runs. The presented results show that the investigated prototype sensors as well as the production process are close to maturity phase for the upgrades of the LHC experiments.

PT14

The pi-transition of the (anti) hydrogen hyperfine structure: improved B-field uniformity for ASACUSA's spin-flip cavity

Martin Simon

Stefan Meyer Institute, Austrian Academy of Sciences, Vienna, AUT, on behalf of the ASACUSA collaboration

In context with ASACUSA's antihydrogen campaign a hydrogen beam experiment has been set up. It was successfully employed for a precise redetermination of the ground-state hydrogen hyperfine splitting (HFS) based on the sigma-transition. This measurement shall be repeated using the π_1 -transition, which is more sensitive to external magnetic fields. Spin-flips are driven in a microwave cavity with stripline geometry. The interaction volume has the shape of a cylinder with a length

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and a diameter of 100mm each. An adjustable uniform guiding-field is required in this region. A McKeehan-type double coil pair served as the starting geometry for the improved magnetic field uniformity. Finite element simulations using the software package COMSOL multiphysics were performed to converge to the optimal coil configuration and to test various shielding geometries. The coils have been manufactured at CERN and the shielding production has been outsourced. Assembly of the components is ongoing. This new setup for pi1 HFS-transitions will be presented.

PT15

A Detector for Measuring the Ground State Hyperfine Splitting of Antihydrogen

Bernadette Kolbinger

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The ASACUSA (Atomic Spectroscopy And Collisions Using Slow Antiprotons) collaboration at the Antiproton Decelerator at CERN aims to test the CPT symmetry by measuring the ground state hyperfine structure of antihydrogen which, according to the theorem of CPT, is predicted to have the same electromagnetic spectrum as hydrogen.

The experimental setup consists of a CUSP trap for antihydrogen production and a Rabi-like spectrometer line consisting of a microwave cavity, a superconducting sextupole magnet and an antihydrogen detector composed of a position sensitive central detector and a hodoscope. This contribution will focus on the two layer hodoscope.

The challenging task of the detector is to discriminate between background events and antiproton annihilations originating from antihydrogen atoms which are produced only in very small amounts. Furthermore, first preliminary results of the 2016 beamtime will be discussed.

PT16

NORM for Building (NORM4BUILDING - COST Project TU-1301)

Harry Friedmann

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This COST initiative stimulates the collaboration of scientists, industries and regulators to gather knowledge, experiences and technologies, to stimulate research on the reuse of residues containing enhanced concentrations of natural radionuclides (NORM) in tailor-made building materials in the construction sector while considering the impact on both external gamma exposure of building occupants and indoor air quality. By improving radiological impact assessment models for the reuse of NORM residues in building materials we hope to further stimulate justified uses of NORM residues in different types of newly developed building materials. Based on these models, we aim at investigating realistic legislative scenarios so that the authorities concerned can allow reuse pathways for NORM that can be accepted from a radioprotection point of view in concordance with the Lead Marked Initiative (LMI) and sustainable construction.

Every year millions of tons of material with an enhanced concentration of natural radioactivity are produced as residues or wastes and usually deposited more or less secure somewhere in the environment:

Metal slags, red mud from the aluminum production, fly ash from coal fire, slag from the phosphor production (fertilizer), industrial gypsum as residues from different chemical industries (e.g. phosphogypsum) and from flue gas desulfurization, oil and gas production, rare earth and zirconium industry, tin, lead and copper melting, mining industry etc. The reuse of such NORM residues can decrease an environmental detriment related to its accumulation at landfills.

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PT17

The VERA facility - AMS with a 3 MV tandem accelerator

Johannes Lachner

Karin Hain, Martin Martschini, Alfred Priller, Peter Steier, Robin Golser

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The Vienna Environmental Research Accelerator VERA is a state-of-the-art facility for accelerator mass spectrometry of trace isotopes. Its central element is a 3MV tandem accelerator. The original setup has been expanded to allow for measurements of ^{10}Be , ^{14}C , ^{26}Al , ^{36}Cl , ^{129}I , ^{236}U , Pu, and other actinide isotopes, which are regularly performed with utmost sensitivities of 10^{-12} to 10^{-16} .

We pursue the introduction and establishment of novel AMS isotopes, which has been successfully demonstrated in the case of ^{236}U . Another focus is set on the development of new techniques for isobar suppression to allow for a measurement of trace isotopes that are to date not accessible to mass-spectrometric determination because of isobaric interferences. In this context an ion cooler is currently integrated into the existing AMS setup to allow for suppression of unwanted isobars by laser photodetachment of the respective negative ion. We will present our established methods for the separation of atomic isobars at VERA and the future prospects with the ion-laser interaction setup along with potential applications of these trace isotopes in environmental sciences (as tracers of water masses, proxy of erosion processes, and dating tools) or in nuclear astrophysics.

PT18

Detection of Pu in Pacific Ocean water by AMS with respect to the Fukushima accident

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The concentration of plutonium (Pu) and its isotopic ratios were determined by accelerator mass spectrometry (AMS) in Pacific Ocean water samples (20 L each) collected in late 2012.

The isotopic ratios $^{240}\text{Pu}/^{239}\text{Pu}$ and $^{241}\text{Pu}/^{239}\text{Pu}$ can be used to identify a possible release of Pu into the ocean by the Fukushima accident. Especially ^{241}Pu ($T_{1/2} = 14.325$ a) is a well-suited indicator for a recent entry of Pu, as ^{241}Pu from fallout of nuclear weapon testings has already significantly decayed. ^{241}Am , the daughter nuclide of ^{241}Pu , causes isobaric background on ^{241}Pu in mass-spectrometric measurements. Therefore, Am and Pu had to be separated chemically using extraction chromatography. The method was verified by analysing the concentration of Pu in certified reference material with AMS at the Maier-Leibnitz-Laboratory in Munich. Ten sea water samples, collected at different depths, were prepared at the Radiochemie München and were measured at the Vienna Environmental Research Laboratory (VERA). A short motivation related to the Fukushima accident, the chemical separation method, and the results of the Pu distribution in the ocean water along with the respective isotopic ratios, obtained in this study, will be discussed. This work was funded by the Studienstiftung des deutschen Volkes.

PT19

PERKEO III - Measurement of the Proton Asymmetry

Michael Klopff (1)

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The semi-leptonic decay of the free neutron is well described within the Standard Model of particle physics (SM). Measurements of observables in neutron decay allow testing the SM and models comprising physics beyond the SM.

The PERKEO III Collaboration performed a measurement of the proton asymmetry parameter C at the Institut Laue-Langenvin (Grenoble, France). The proton asymmetry describes the angular correlation between the momentum of the decay proton and the spin of the neutron. In the SM, the decay of the free neutron is covered within the framework of V-A theory. All neutron decay parameters, including the proton asymmetry, depend only on the ratio of axial-vector (g_A) to vector coupling constant (g_V). Deviations from SM expectations would give a hint on additional couplings such as scalar or tensor couplings.

On our poster we will present the measurement principle with the focus on systematic effects of the PERKEO III experiment, and give first estimates for the systematic corrections. Systematic effects are mainly caused by shape and magnitude of the magnetic and electric fields, the shape of the neutron beam and the limited size of the detectors.

PT20

From the stars through the ocean abyss: the long travel of super-nova Pu-244 into VERA's particle detector

Peter Steier (1)

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Half of the nuclides in the cosmos heavier than iron - including all actinides - are generated in explosive environments by r-process nucleosynthesis. However, the relevant astrophysical sites, and the history of the r-process during the Galactic chemical evolution remain a mystery. With a half-life of 81 My, ^{244}Pu can place strong constraints on recent r-process frequency and production yield. ^{244}Pu from recent nucleosynthesis can reach the Earth in two ways: a relatively close supernova may inject it to our planet directly, or the shock front of the explosion may

sweep up ^{244}Pu accumulated in interstellar dust and transport it to Earth. We have carried out a search for live interstellar ^{244}Pu in deep-sea reservoirs [1], which are expected to accumulate interstellar dust particles over long time periods. The Accelerator Mass Spectrometry (AMS) facility VERA at the University of Vienna was optimized and extended over the years for the detection of actinides. ^{244}Pu can be detected practically without instrumental background and high sensitivity.

Two kinds of deep-sea archives were investigated: with a growth rate of a few millimeter per million years, hydrogenous crusts will strongly concentrate elements and particles. The higher accumulation rate of deep-sea sediments (mm/ky) results in a better time resolution but requires much larger sample volumes. We used a deep-sea manganese crust (237 KD from cruise VA13/2, collected in 1976) with a growth rate between 2.5 mm per My and 3.57 mm per My; it originates from the equatorial Pacific at a depth of 4,830 m and covers the last 25 My. Our second sample, also from the Pacific Ocean, is a piston-core deep-sea sediment (7P), extracted during the TRIPOD expedition as part of the Deep-Sea Drilling Project (DSDP) at 3,763 m water depth and covers a time period of about 0.5–2.1 My before present.

The plutonium was extracted from 12 individual pieces with masses between 30 and 360 g. The AMS measurement procedure was a sequence of alternating counting periods of ^{236}Pu or ^{242}Pu yield tracer, ^{239}Pu , and ^{244}Pu . All samples were repeatedly measured until they were completely exhausted, and lasted 5 to 20 hours. The overall yields for the 12 crust samples were between 0.06×10^{-4} and 1.54×10^{-4} . Reference samples containing a well-known isotope ratio of $^{244}\text{Pu}/^{242}\text{Pu}$ reproduced the nominal values within 4%. A clear anthropogenic ^{239}Pu and ^{244}Pu signal, originating from atmospheric atomic-bomb tests from ca. 1950 to 1963, was observed in the top layer of the deep-sea manganese crust (16 events of ^{244}Pu detected). However, only two atoms of ^{244}Pu were detected in the deeper layers of the crust sample, and one in the sediment. This is two orders of magnitude less than expected from continuous production in the Galaxy. Our findings indicate that ^{244}Pu has not accumulated to a steady state in the interstellar matter, and thus supernovae did not contribute significantly to actinide nucleosynthesis for the past few hundred million years. Actinide nucleosynthesis, as mapped through live ^{244}Pu , seems to be very rare.

[1] A. Wallner, T. Faestermann, J. Feige, C. Feldstein, K. Knie, G. Korschinek, W. Kutschera, A. Ofan, M. Paul, F. Quinto, G. Rugel, P. Steier. Abundance of live Pu-244 in deep-sea reservoirs on Earth points to rarity of actinide nucleosynthesis. *Nature Communications* 6:5956 (2015)

PT31

A cold neutron beam facility for particle physics at the ESS

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Pulsed beams have tremendous advantages for precision experiments with cold neutrons. In order to minimise and measure systematic effects, they are used at continuous sources in spite of the related substantial decrease in intensity. At the pulsed neutron source ESS, such experiments will gain up to a factor of 30 in event rate, and novel concepts become feasible. Therefore, the cold neutron beam facility for particle physics ANNI was proposed as part of the ESS instrument suite. Scientific case, concept and expected performances of ANNI will be presented.

PT32

Design of the Magnetic Shielding for NoMoS

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The new instrument NoMoS is a novel type of momentum spectrometer, currently under development at the Stefan Meyer Institute. Its main component is an R×B magnet which determines the momentum of charged particles by their drift in a circular magnetic field (about 150 mT). First measurements with neutrons are planned at the Institut-Laue-Langevin in Grenoble/France. For measurements at ultimate statistics, NoMoS will be installed at PERC (up to 6 T), a new facility at the FRM II in Garching/Germany. In order not to disturb other experiments in the vicinity of NoMoS, we have designed a variable magnetic shielding.

The finite element method (COMSOL Multiphysics) has been used to determine the most suited geometry for the shielding. The following considerations were taken into account: the magnetic stray field is suppressed to the cardiac pacemaker level (0.5 mT at less than 2.5 m), the internal magnetic field and its homogeneity (around 10^{-4}) are not disturbed, the additional forces onto the coils are not destructive, and the shielding deals with the limited space conditions (max. width 5 m). For experimental reasons, the magnet geometry is non-axisymmetric and therefore has to be simulated in 3D. To reduce the computing time and simultaneously increase the numerical accuracy, we simulated only one half of the geometry, taking advantage of the symmetry both of magnet and shielding. However, to study the influence of the shielding on the particle trajectories we had to simulate the full geometry. The design of the magnetic shielding for NoMoS will be presented.

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PT21

Dating Kaali Crater (Estonia) based on charcoal emplaced within proximal ejecta blanket.

Eva Maria Wild (1)

Anna Losiak (2,3), Anna Losiak (3), T. Wisniowski (4), K. Paavel (5), A. Joeleht (6), R. Välja (6), J. Plado (6), A. Kriiska (5), J. Wilk (7), M. Zanetti (8), W. D. Geppert (9), A. Kulkov (10), Peter Steier (1), I. Pirkovic (11), M.S. Huber (12)

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The Kaali impact field consists of nine identified craters located on the Saaremaa Island in Estonia. The largest crater is 110 m in diameter (centered around 58°22'21.94"N, 22°40'09.91" E). It was formed by impact of an IAB iron meteoroid into Silurian dolomite target rocks covered by up to a few meters of glacial till (Veski et al. 2007). The age of the Kaali impact structure is still a matter of debate, and the estimates provided by different authors vary considerably between ~6400 BC (Raukas et al. 1995, Moora et al. 2012) and ~400 BC (Rasmusen et al. 2000, Veski et al. 2001). These ages were derived by ¹⁴C dating of marker horizons, characterized by a slightly elevated iridium content within the nearby Piila bog yielding a calibrated age of 800-400 BC (Rasmussen et al. 2000, Veski et al. 2001) and occurrences of glassy siliceous material in the Piila bog (~6400 BC: Raukas et al. 1995) or iron microspherules in an organic-rich layer of the Reo gravel pit (6400 BC: Moora et al. 2012). However,

the source of the foreign material within those layers was never unequivocally connected with the Kaali crater. ¹⁴C dating of material from post-impact organic sediments within Kaali impact craters yielded ages between 1800-1500 BC (Saarse et al. 1991, Veski et al. 2004) and 1450-400 BC (Aaloe et al. 1963). These dates underestimate the age of impact as organic sediments within the crater started to form at unknown period after the impact. On the other hand, Veski et al. (2004) suggested a reservoir effect that might have caused artificially “aging” of the organic matter because the crater was emplaced within Silurian dolomite which is rich in old carbon. The aim of this study is to determine the age of the Kaali crater by ¹⁴C dating of organic material covered by the continuous layer of proximal ejecta. This research was conducted in conjunction with a new structural investigation of Kaali Main Crater (Zanetti et al. 2015).

Thirteen samples collected from different locations within the trench (located ~12 meters to the SW from the rim crest of the main crater) and at different depths in respect to the ejecta-till boundary were processed separately. ¹⁴C dating was performed at the Vienna Environmental Research Accelerator at the University of Vienna (Austria). The calibrated (95,4% probability) time ranges of 11 out of 13 samples span the time interval from ~1650 BC to ~1400 BC. This age is based on dating charcoal within the ejecta blanket which makes it directly linked with the impact structure, and not susceptible to potential reservoir effects.

Results of this study are published in Losiak et al, 2016.

Aaloe et al. 1963. *Eesti Loodus* 6:262-265.
 Moora et al. 2012. *Geochronometria* 39: 262-267.
 Raukas et al. 1995. *Proc. Estonian Acad. Sci., Geology* 44:177-183.
 Rasmussen et al. 2000. *MAPS* 35:1067-1071.
 Saarse et al. 1991. *Bull. Geol. Soc. Finland* 63:129-139.
 Veski et al. 2007. *Comet/Asteroid Impacts and Human Society*:265-275.
 Veski et al. 2001. *MAPS* 36:1367-1376.
 Veski et al. 2004. *Veg Hist Archaeobot* 13:197-206.
 Zanetti et al. 2015. 46th LPSC.
 Losiak et al, 2016 *MAPS* 51, Nr 4, 681–695

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Investigation of transitions conditioned by temperature and composition change in a 4 component lipid-only system

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Membranes, as they occur in mammalian cells, are as interesting as they are complex. Therefore, simple models have to be found to understand their behavior and subsequently use this knowledge for various health applications like drug therapy.

Building artificial membranes of lipid-only systems to study their properties under controlled and simplified conditions is a well-established method in the field of biophysics. This contribution focusses on DSPC/DOPC/POPC/Cholesterol mixtures, which generate domain structures of coexisting liquid-ordered (Lo) and liquid-disordered (Ld) phases.

The first aspect investigated is the dependence of the domain size on the DOPC/POPC ratio, particularly the transition from macroscopic to nanoscopic domains with increasing POPC content. Small Angle X-ray Scattering (SAXS) data were collected at different synchrotron facilities and further analyzed with a global analysis program for multilamellar vesicles. This novel approach allows for parameters such as the bilayer thicknesses and the bending fluctuations to be determined. Furthermore our compositional data suggests that the critical behavior follows a 2-dimensional Ising Model.

Secondly, SAXS and Differential Scanning Calorimetry (DSC) measurements monitored the temperature dependence of the transition between a domain structure (phase separation) and a homogeneous Ld phase. Our data provides insight into the melting of Lo domains, showing a dependence of the transition temperature on the DOPC/POPC ratio. Notably, a shift to higher temperatures with increasing DOPC content is observed.

This work was supported by Austrian Science Fund FWF, Project No. P24459-B20.

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Detection of anthropogenic ¹²⁹I to approach sediment dynamics in the Kaunertal valley

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¹²⁹I is a long-lived radionuclide that has been introduced into the environment as a consequence of atmospheric nuclear bomb explosions and reprocessing of nuclear fuel. Its environmental abundance provides information on the relative time of formation of water bodies. We determined ¹²⁹I concentrations with accelerator mass spectrometry at the Vienna Environmental Research Accelerator VERA from sample volumes of 0.5L precipitation, spring water, glacier melt water, and rivers. This allowed the relative dating of evolving spring waters in lateral moraines of the Gepatschferner glacier in the Upper Kaunertal. This glacier has undergone large deglaciation processes in the past decades, which has left behind large lateral moraines that are now exposed to erosion. Our results allow the attribution of the spring water to modern precipitation, old dead ice, or to mixing of sources of different age.

PT24

Confocal SR- μ XRF measurements of increased Zinc accumulation in mineralized osteosarcoma

Mirjam Rauwolf (1)

Bernhard Pemmer (1), Andreas Roschger (2), Anna Turyanskaya (1), Stephan S. Smolek (1), Angelika Maderitsch (1), Peter Hischenhuber (1), Martin Foelser (1), Rolf Simon (3), Susanna Lang (4), Stephan E. Puchner (5), Reinhard Windhager (5), Klaus Klaushofer (2), Peter Wobrauschek (1), Paul Roschger (2), Jochen G Hofstaetter (6), Christina Strelj (1)

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Vienna General Hospital, Vienna, AUT (5) Department of Orthopaedic Surgery, Vienna General Hospital, Vienna, AUT (6) Orthopaedic Hospital Vienna-Speising, Vienna, AUT

Abnormal tissue levels of certain trace elements such as Zinc (Zn) were reported in various types of cancer. Little is known about the role of Zn in osteosarcoma.

Using confocal synchrotron radiation micro X-ray fluorescence analysis, we characterized the spatial distribution of Zn in high-grade sclerosing osteosarcoma of nine patients following chemotherapy and wide surgical resection. Zn levels in mineralized osteosarcoma tissue were compared to levels in adjacent normal tissue. Quantitative backscattered electron imaging (qBEI) as well as histological examinations were also performed.

On average, the ratio of medians of Zn count rates (normalized to calcium) in mineralized tumor tissue was about 6 times higher than in normal tissue. There was no difference in Zn levels between tumor fraction areas with a low and a high fraction of mineralized tissue, which were clearly depicted using qBEI. Moreover, we found no correlation between the Zn values and the type of tumor regression according to the Salzer-Kuntschik grading.

The underlying mechanism of Zn accumulation remains unclear. Given the emerging data on the role of trace elements in other types of cancer, our novel results warrant further studies on the role of trace elements in bone cancer.

PT25

Confocal μ XRF spectrometer for analysis of 3-dimensional spatial distribution of low to high Z elements

Lukas Perneczky

Anna Turyanskaya, Mirjam Rauwolf, Stephan Smolek, Peter Wobrauschek, Christina Strelt

Atominstytut, TU Wien, Vienna, AUT

Confocal μ XRF is a powerful tool for analyzing the spatial distribution of major, minor and trace elements in 3 dimensions. Being a non-destructive analyzing technique, confocal μ XRF is suited for measuring a wide

spectrum of samples (biological, geological, cultural heritage, etc.). The ATI's μ XRF spectrometer uses a low power tube with Rh anode (20 W) as excitation source. In order to focus the primary beam onto the sample, a polycapillary full-lense (XOS) with a nominal spot-size of $32\mu\text{m}$ for Mo Ka is installed between tube and sample stage. For confocal measuring, a polycapillary half-lense (XOS) can be mounted between sample and detector. Both polycapillary lenses are mounted on piezo positioner xyz-stacks (Attocube) to make for a convenient adjustment procedure. Fluorescence radiation is detected by a 30mm^2 LN2 cooled Si (Li) detector with an ultra-thin polymer window to minimize absorption of low Z element fluorescence lines. Additionally, the whole setup is situated in a vacuum chamber (~ 1 mbar), making it perfectly suited for measuring low Z elements. The sample is mounted on a motorized xyz stage and for precise positioning of the sample, an optical video microscope is focused on the z-position of the confocal volume, while the xy- position is marked by an adjustable ellipse on the microscope screen.

The μ XRF spectrometer can be operated in non-confocal (with only one lens in the excitation channel, i.e. conventional μ XRF) or confocal (with a second lens between tube and sample) mode. In confocal μ XRF, two focussing optics are adjusted such, that their beam paths are intersecting. Consequently, the detected fluorescence radiation is coming solely from this confocal volume, allowing the determination of the spatial distribution of elements in a sample in 3 dimensions. For the confocal setup a voxel size of $50\mu\text{m} \times 50\mu\text{m} \times 50\mu\text{m}$ for Cu-Ka was determined. Line-, area- and volume-scans can be programmed using the in-house μ XRF-software package. Line-scans can be utilized for depth scans, while area-scans provide elemental maps of a sample. Here, the confocal setup has the advantage over elemental maps created by conventional μ XRF, with better spatial resolution and higher surface sensitivity. Furthermore, volume scans enable the user to measure 3-dimensional element distributions. The setup will be presented together with exemplary measurements.

PT26

Total X-ray reflection fluorescence spectrometry analysis of trace elements in tea and herbal infusions

Aleksandra Winkler

Mirjam Rauwolf, Anna Turyanskaya, Johannes Sterba, Peter Wobrauschek, Christina Streli

Atominstytut, TU Wien, Vienna, AUT

The aim of this study was to determine elemental composition including trace element content in the various tea and herbal infusions, among them those which are used for medical treatment purposes, by the mean of Total Reflection X-ray Fluorescence Analysis (TXRF). TXRF is an energy dispersive X-ray fluorescence (EDXRF) method with a special geometry, which is known for and characterized by its easy sample preparation, especially for solutions, simple quantification and increased elemental measurement sensitivity, compared to conventional EDXRF. Using the Mo-W mixed alloy anode X-ray tube the samples were monochromatically excited by Mo K α energy. The measurements were conducted under ambient conditions. The fluorescence radiation emitted from tea samples was analyzed with Si (Li) - detector with 80 mm² area, with 12 μ m Beryllium window. The tube voltage and current were constant during the whole measurement process - 50 kV and 37 mA. During this work the observation was made which elements can be called intrinsic for the certain tea/herbal solution type and which are more accidental, caused by pollution, soil difference or similar. It is essential to know elemental composition of a tea, due to high consumption [1] of this drink. The separate elements can relieve some disease symptoms or even pain. Some can cause serious health issues when overdosed. For example, phosphorous can increase the risk of cardiovascular disease [2].

The methodology of sample preparation was developed and data from 29 teas and herbal solutions were collected. Evaluation and comparison between different types of tea/herbal solution were made based on statistically treated data and will be presented.

[1] <http://www.thie-online.eu/herbal-infusions/herbal-infusions-history/>

[2] <http://umm.edu/health/medical/altmed/supplement/phosphorus>

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PT27

Optimization of inverted hexagonal lipid phase preparation by the rapid solvent exchange

Neda Negahbani

Santosh Prasad Gupta, Drew Marquardt, Georg Pabst

Institute of Molecular Biosciences, University of Graz, Graz, AUT

We have tried for the first time to make the inverted hexagonal structure (H_{II}) of different lipid mixtures by the rapid solvent exchange (RSE) method. In this process a host lipid was mixed with lipids composed of different carbon chain lengths. The host and guest lipids were dissolved separately in the organic solvent before mixing together. The organic solvent was removed during RSE process of producing an organic-solvent free mixture of the host and guest lipids. Each sample was investigated by the small angle x ray scattering (SAXS) at different temperatures. We have found the lattice parameter and spontaneous curvature of samples by in-house Matlab codes. Our results showed this approach can yield to make the net H_{II} lipid structures. Therefore, using the RSE can help to make lipid mixture in H_{II} phase in a timely fashion. Also, for each examined bilayer forming lipid, the spontaneous curvature of the pure monolayer structure was found by the extrapolation. According to our results, there is no correlation between spontaneous curvature and the lipids carbon chain length.

PT28

New Particle Formation in Urban Atmospheres: Comparison between Vienna, Prague and Budapest and Influence of Air Mass Origin

Bernadette Rosati (1)

N. Zíková (2), A. Wonaschütz, (1), C. Dameto de Espana (1), G. Steiner (1,3), V. Zdimal (2) J. Schwarz (2), T. Weidinger (4), I. Salma (5), R. Hitzemberger (1)

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Physics, University of Innsbruck, Innsbruck, AUT (4) Department of Meteorology, Eötvös University, Budapest, HUN (5) Institute of Chemistry, Eötvös University, Budapest, HUN

New particle formation (NPF) leads to high number concentrations of ultrafine particles, which can further grow to become relevant for cloud formation and may also affect air quality and public health. Several studies focused on NPF events in different urban places, including detailed investigations in Vienna, Prague and Budapest. Particle size distributions together with gaseous precursors and local meteorology were also explored extensively in these cities. The origin of the air masses arriving at a certain location may play a role for NPF as it modifies the particle concentrations (clean vs. polluted air masses) but also chemical composition (see e.g. Wonaschütz et al., 2015). In this study, aerosol particle size distributions from 2014 and 2015 measured in Vienna, Prague and Budapest are compared. All three cities are situated in Central Europe in proximate vicinity (distance between Prague and Vienna: 250 km; Vienna and Budapest: 220 km; Prague and Budapest: 440 km) and have about 1.5 million inhabitants each. Due to these similarities, it is possible that the characteristics of NPF events might be comparable in the three cities and that NPF events may occur concurrently. The scope of this work is to test the three cities for simultaneous NPF events. The study focuses on NPF event days occurring in all three cities and on days when NPF events occurred only in two out of three cities. Air mass origins were modeled using the HYSPLIT back-trajectory model (Stein et al., 2015) with the GDAS system providing meteorological data with a resolution of 0.5°. First results show inter-annual variations in NPF frequencies with most concurrent NPF events in spring and summer. While in 2015, such days were mostly associated with north-westerly air masses, the picture is more complex in 2014 with no clear predominant wind direction on simultaneous NPF days. Additionally, differences between the cities appear quite striking and lead to only very few instances with concurrent NPF events. Closest resemblance can be found between results in Budapest and Prague, whereas Budapest and Vienna show the most differences.

Stein, A.F., Draxler, R.R., Rolph, G.D., Stunder, B.J.B., Cohen, M.D., and Ngan, F., NOAA's HYSPLIT atmospheric transport and dispersion modeling system, Bull. Amer. Meteor. Soc., 96, 2015, 2059-2077, <http://dx.doi.org/10.1175/BAMS-D-14-00110.1>

Wonaschütz, A., Demattio, A., Wagner, R., Burkart, J., Zíková, N., Vodička, P., Ludwig, W., Steiner, G., Schwarz, J., Hitzemberger, R., Seasonality of new particle formation in Vienna, Austria – Influence of air mass origin and aerosol chemical composition, *Atmospheric Environment*, Volume 118, 2015, Pages 118-126, ISSN 1352-2310, <http://dx.doi.org/10.1016/j.atmosenv.2015.07.035>.

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PT29

Entanglement Entropy in Heavy Ion Collisions

Philipp Stanzer

TU Wien, Vienna, AUT

Using the methods of holography we calculate the two-point function and entanglement entropy in heavy ion collisions, modeled by colliding gravitational shock waves in Anti-de Sitter spacetime.

Using two different initial conditions, wide and narrow shock waves, we find qualitatively different behavior of the calculated quantities. This allows to use the entanglement entropy as order parameter to distinguish between the transparency and full stopping scenario of colliding shock waves.

PT30

Causally nonseparable processes admitting a causal model

Adrien Feix

Mateus Araújo, Caslav Brukner

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A recent framework of quantum theory with no global causal order predicts the existence of “causally nonseparable” processes. Some of these processes produce correlations incompatible with any causal

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order (they violate so-called “causal inequalities” analogous to Bell inequalities) while others do not (they admit a “causal model” analogous to a local model). Since the only processes known to be physically implementable have a causal model, it is tempting to conjecture that having a causal model singles out physically realizable processes. Here we provide evidence against this conjecture. We show for the first time that bipartite causally nonseparable processes with a causal model exist, and argue that they have no clear physical interpretation. We also provide an algorithm to generate processes of this kind and show that they have nonzero measure in the set of all processes. Finally, we demonstrate the existence of processes which stop violating causal inequalities but are still causally nonseparable when mixed with a certain amount of “white noise”. This is reminiscent of the behavior of Werner states in the context of entanglement and nonlocality. This is an SFB-FoQuS submission.

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17:15-18:45

**3rd Floor
in front of Josef-Stefan-Hörsaal**

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PW01

Stabilization of deformation induced lattice defects in hydrogenated palladium subjected to severe plastic deformation

Wolfgang Reß (1)

Daria Setman (1), Andreas Grill (1), Erhard Schafner (1), Wolfgang Sprengel (2), Yuzeng Chen (3), Michael Zehetbauer (1)

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Recently it has been shown that in hydrogenated and SPD (Severe Plastic Deformation) processed palladium the densities of lattice defects, i.e. dislocations and vacancies, were significantly higher than without hydrogenation [1], because of the stabilization of the defects through the hydrogen absorbed. Further investigations of the authors showed that these enhanced densities of lattice defects caused an enormous hardening [2, 3, 4]. The results tend to be in line with previous investigations by Chen et al. [2] claiming that all the hardening arises solely from the hydrogen induced enhancement of dislocation density. In order to carefully check this result, isochronal microhardness measurements

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have been undertaken which allowed to separate the specific strength contributions (if any) arising from vacancies (vacancy agglomerates), from dislocations and perhaps further ones from grain boundaries. To quantify the actual concentrations and sizes of lattice defects, the methods of DSC and PAS (Differential Scanning Calorimetry, Positron Annihilation Spectroscopy, both being sensitive to vacancy defects and dislocations), and of XPA (X-Ray Bragg Profile Analysis, being sensitive to dislocations only) were applied in parallel to the microhardness measurements. Surprisingly it was found that the major part of hardening arises from the vacancies (vacancy agglomerates) and only a smaller one from the dislocations, while there was no effect from varying grain size.

Financial support by the FWF (Austrian Science Fund) in frame of project T512-N20 is gratefully acknowledged.

[1] M. Krystian, D. Setman, B. Mingler, G. Krexner, M.J. Zehetbauer, *Scripta Mater.* (2010) 49

[2] Y. Z. Chen, H.P. Barth, M. Deutges, C. Borchers, F. Liu, R. Kirchheim, *Scripta Mater.* 68 (2013) 743

[3] D. Setman, W. Röss, A. Grill, E. Schafner, Y.Z. Chen, R. Kirchheim, M. Zehetbauer, Lecture at the Int.Conf. THERMEC 2016 (Graz, Austria)

[4] K. Werbach, M. Deutges, Y.Z. Chen, A. Grill, D. Setman, G. Krexner, R. Kirchheim, M. Zehetbauer. Lecture at the Int.Conf. HySEA 2014 (Rio de Janeiro, Brasil)

PW02

Slow dynamics of supercooled water in nano-confinement

Viktor Soprunyuk (1)

Patrick Huber (2)

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Dynamical mechanical analysis (DMA) ($f=0.2 - 100$ Hz) is used to study the dynamics of confined water in mesoporous Gelsil (2.6 nm and 5 nm pores) and Vycor (10 nm) in the temperature range from 80 K to 300 K [1]. Confining water into nanopores partly suppresses crystallization

and allows us to perform measurements of supercooled water below 235 K, i.e. in water's so called „no man's land“. Two relaxation peaks are observed in $\tan \delta$ around 140 K (P1) and 205 K (P2) for Gelsil 2.6 nm and Gelsil 5 nm at 0.2 Hz shifting to higher temperatures with increasing pore size d . They change with frequency in a systematic way, due to an Arrhenius behaviour of the corresponding relaxation times.

It is suggested that P1 corresponds to the glass transition of supercooled water far from pore walls, whereas P2 reflects the dynamics of water molecules near the surface of the pores. The observation of a clear softening of the Young's modulus around 165 K (for Gelsil 2.6 nm at 0.2 Hz) is in agreement with a glass to liquid transition in the vicinity of P1. We find a distinct $1/d$ -dependence of the glass transition temperature [2]. An extrapolation to $1/d \rightarrow 0$ suggests that the glass transition temperature of bulk water takes the traditional value of 136 K.

PW03

Quartic scaling MP2 for extended systems: A step towards vertex corrections.

Tobias Schäfer

Georg Kresse

Faculty of Physics, University of Vienna, Vienna, AUT

A standard approach in computational quantum chemistry to evaluate the energy of matter is to use Hartree-Fock (HF) theory and approximate the correlation energy in second order by applying Moeller-Plesset perturbation theory (MP2). However, conventional MP2 implementations scale with the fifth power in the number of electrons (N^5) and are therefore very costly for large systems. Here we present a new implementation that has a lower scaling (N^4) and a very high parallelization efficiency. It is based on the Laplace transformation, or equivalently on a description of perturbation theory in imaginary time. It is worthwhile mentioning that the algorithm can be adapted to calculate second order screened exchange (SOSEX) as well as the particle-hole ladder diagrams with a similar low complexity.

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PW04

Magnetic and electrostatic hyperfine interactions in FeSb₂

Michael Reissner

Klaudia Hradil, Walter Steiner

TU Wien, Vienna, AUT

Because of its colossal Seebeck coefficient [1] and its rather high charge carrier mobility [2], FeSb₂ is a candidate for several interesting applications like thermoelectrics and high speed electronics. Magnetically FeSb₂ shows a quite unusual behaviour. At low temperatures susceptibility is constant with a value near to zero, pointing to a nonmagnetic ground state. Above approximately 90 K susceptibility increases and magnetization curves point to paramagnetic behaviour. This temperature induced magnetism is usually explained either by a small gap insulator with an semiconductor – metal transition around 90 K [3] or by a near ferromagnetic ground state [4]. FeSb₂ crystallizes in the marcasite structure type with only one crystallographic Fe site. The Fe is surrounded by slightly distorted Sb octahedra, which are corner shared in the ab-plane and edge sharing along the c-axis. The distortion is a squeezing of the octahedron along the apical axis. This is in good agreement with ⁵⁷Fe Mössbauer measurements, which can be explained by only one subspectrum. In contrast to this, Mössbauer spectra taken in external magnetic fields cannot be explained by only one subspectrum. The obtained spectra are extremely complex [5]. Several subspectra are necessary to explain the measured spectrum. From a thorough structural investigation by X-ray and neutron diffraction measurements it is concluded that approximately 30% of the Fe atoms are shifted out of the center of the octahedron. A closer look to the structure shows that the two Fe atoms in the unit cell, which are in the average structure crystallographically identical, are not the same in case of the electronic structure, because the apical axis of the octahedra is not perpendicular to the basal plane but tilted by approximately two degrees. The distortion of the Sb octahedron as a consequence of the off-site position of part of the Fe atoms lead to distribution of isomer shift, large spread in quadrupole splitting and rather large asymmetry parameter. Analysis of the magnetic hyperfine fields show that those Fe atoms which are still

in the center of the octahedrons have no hyperfine field, whereas those shifted out of the center show a small ferromagnetic like hyperfine field.

[1] Bentien A et al, 2007 EPL 80 17008

[2] Hu R et al, 2008 APL 92 182108

[3] Petrovic C et al, 2003 Phys. Rev. B 67 155205

[4] Lukoyanov A V et al, 2006 Eur. Phys. J. B 53 205

[5] Farhan A et al, 2009 J. Phys. Conf. Ser. 215 012142

PW05

Ionic microgels under the influence of AC electric fields: theory and simulations

Thiago Colla (1)

Christos N. Likos (2)

(1) Universidade Federal do Rio Grande do Sul, Porto Alegre, BRA (2) Faculty of Physics, University of Vienna, Vienna, AUT

When subject to an alternating electric field, ionic microgels get polarized due to the resulting ionic diffusion both inside and outside their polymer networks. The ionic response can be described by the build-up of an effective microgel dipole moment, whose magnitude can be controlled by the strength of the applied field. As a consequence, the ionic-averaged microgel interactions comprise a dipole-dipole interaction in addition to the usual monomer screened potential. Recently, a series of experiments have been performed in the high-frequency domain, revealing a rich class of structural transitions driven by the field-induced interactions. In the present work, a coarse-graining model is proposed to describe the effective interactions between ionic microgels under the influence of a high-frequency electric field. The resulting interactions are then used in combination with Integral Equations theory and Molecular Dynamic simulations in order to describe the structural features observed experimentally.

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PW06

Dynamics enhanced by HCl doping triggers full Pauling entropy release at the ice XII/XIV transition and its isotope effect

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The pressure–temperature phase diagram of ice displays a perplexing variety of structurally distinct phases. In the century-long history of scientific research on ice, the proton-ordered ice phases numbered XIII through XV were discovered only recently. Despite considerable effort, none of the transitions leading from the low-temperature ordered ices VIII, IX, XI, XIII, XIV and XV to their high-temperature disordered counterparts were experimentally found to display the full Pauling entropy. Using calorimetric measurements on suitably high-pressure-treated, hydrogen chloride-doped ice XIV we demonstrate just this at the transition to ice XII. Dielectric spectroscopy on undoped and on variously doped ice XII crystals reveals that addition of hydrogen chloride, the agent triggering complete proton order in ice XIV, enhances the precursor dynamics strongest. These discoveries provide new insights into the puzzling observation that different dopants trigger the formation of different proton-ordered ice phases.

This is the first time in 100 years of research on ice that a transition from full disorder to full order could be achieved. The theoretical possibility of this was envisioned in 1935 by Linus Pauling, and only 80 years later his vision came true.

Likewise, a calorimetry study of the isotope effect in the transition from ice XII to ice XIV has been done, with the goal of understanding the low-temperature dynamics in water. Using DCl as a dopant agent and demonstrate how the deuterated ice XII slows the dynamics with a change in the onset temperature of conversion of ~5K and how the possibility of a 100% proton-order ice XIV, becomes more difficult. Due to the change in mass H/D, we believe this strong isotope effect is due to quantum effects.

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PW07

Comparison of results of different methods to investigate the pinning behaviour of superconductors

Michael Reissner (1)

Boris Brunner (2), Clara Boder (1), Pavol Kovac (2), Chao Yao (3), Xianping Zhang (3), Yarwei Ma (3)

(1) TU Wien, Vienna, AUT (2) Slovak Academy of Sciences, Bratislava, SVK (3) TU Wien, Vienna, AUT (4) Chinese Academy of Sciences, Beijing, CHN

The knowledge of the mechanisms which lead to high critical current densities are important for the development of new preparation routes. As for classical metallic superconductors the scheme of Dew-Hughes [1] for strong pinning centres works good, it often fails for the new superconductors. Reason is, that these new superconductors have either weak pinning centres and/or much richer phase diagrams, where pinning mechanisms change with changing temperature and field, which makes analyses within the Dew-Hughes scheme complicate. For the oxid high temperature superconductors analysis of pinning behaviour in terms of the collective creep theory was shown to work well (e.g. [2]). The analysis of magnetic relaxation measurements within the scheme of Maley et al. [3] allows to determine the $U(J)$ -relation, where U is the effective pinning energy and J the current density. From these the different pinning regimes can be identified. For MgB₂ and the iron containing pnictides the situation is not as clear, which analysis is better. In this paper we will discuss the results of different analyses of magnetic relaxation measurements especially for MgB₂ and 122-pnictide superconductor.

[1] D. Dew-Hughes, Phil.Mag. 30 (1974) 293

[2] M. Reissner and J. Lorenz Phys. Rev. B 56 (1997) 6273

[3] M.P. Maley, J.O.Willis, H. Lessure, and M.E. McHenry, Phys.Rev. B 42 (1990) 2639

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PW08

Commensurability of magnetic flux quanta with artificial defect arrays in cuprate superconductors probed by critical current, magnetoresistance, and Hall Effect

Georg Zechner (1)

Lisa Haag (1), Florian Jausner (1), Wolfgang Lang (1), Meirzhan Dosmailov (2), Marius Bodea (2), Johannes Pedarnig (2)

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The interaction of vortices with artificial defects in a superconductor is a topic of intense interest; from the viewpoint of fundamental experimental and theoretical research, as well as from the prospect of technical applications [1]. In contrast to clean metallic superconductors that were often used to study regular artificial defects, the typical average distance of random intrinsic defects in a prototypical cuprate superconductor, namely $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) is about 300 nm. Therefore, only with the emergence of advanced nanopatterning methods that allow for the fabrication of regular arrays of many thousands of defect columns with (sub)- μm distance in a thin superconducting film [2] it became possible that artificial structures can compete with the strong intrinsic pinning in these materials.

YBCO thin films on MgO substrate were irradiated with He^+ ions by shadow projection through a Si stencil mask to create a square array of cylindrical defect regions with 300 or 500 nm lattice constant, respectively [3]. In a field-cooled experiment, distinct peaks of the critical current as a function of the applied magnetic field can be observed in a wide temperature range, when the density of magnetic flux quanta is commensurate with the density of the defect columns [4]. At the same magnetic fields, the magnetoresistance exhibits minima. If the sample is zero-field cooled and then the magnetic field is swept up and down, both peaks and minima show a pronounced hysteresis that leads to an offset of the matching signatures from their field-cooled values. Interestingly, the distances of the various peaks or minima in a sweep remain constant and correspond exactly to the matching field.

Measurements of the vortex Hall effect reveal a novel vortex commensurability behavior, a sign reversal of the Hall effect that occurs only at a

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magnetic field corresponding to the occupation of every defect column by exactly one flux quantum. We attribute this observation to a change of the vortex pinning at the matching field.

1. V.V. Moshchalkov, R. Wördenweber, W. Lang (eds.), Nanoscience and Engineering in Superconductivity, Springer 2010.
2. W. Lang, M. Dineva, M. Marksteiner, T. Enzenhofer, K. Siraj, M. Peruzzi, J.D. Pedarnig, D. Bäuerle, R. Korntner, E. Cekan, E. Platzgummer, H. Loeschner, Microelectronic Engineering, 83, 1495 (2006).
3. J.D. Pedarnig, K. Siraj, M.A. Bodea, I. Puica, W. Lang, R. Kolarova, P. Bauer, K. Haselgrübler, C. Hasenfuss, I. Beinik, C. Teichert, Thin Solid Films 518, 7075 (2010).
4. L.T. Haag, G. Zechner, W. Lang, M. Dosmailov, M. A. Bodea, J. D. Pedarnig, Physica C 503, 75 (2014).

This work was supported by the COST Action MP1201, Nanoscale Superconductivity: Novel Functionalities through Optimized Confinement of Condensate and Fields (NanoSC -COST)

PW09

B-doped SWCNTs as part of a new generation of materials in semiconductor industry

Carlos Reinoso (1)

Kazuhiro Yanagi (2), Philip Rohringer (1), Thomas Pichler (1), Paola Ayala (1,3)

(1) Faculty of Physics, University of Vienna, Vienna, AUT (2) Tokyo Metropolitan University, Tokyo, JPN (3) Yachay Tech University, Urququi, EC

Incorporating heteroatoms such as Boron as „dopants“ in the crystal-line lattice of a single-walled carbon nanotube (SWCNT) induces changes in its intrinsic properties. Understanding the bonding environment of the dopants and their distribution in the wall of B-doped SWCNTs is crucially important for applications. However, the tubes´ heterogeneity, their bundling, and the presence of catalytic by-products hinder their direct application. We have optimized the production of SWCNTs doped with B using a high-vacuum assisted chemical vapour deposition method developed in-house and this work shows our progress regarding the subsequent purification processes we have tried. The density

gradient ultracentrifugation method has been investigated in this work as an alternative to the conventional chemical purification treatment that could possible affect to the functionalized material. In order to characterize this material, multifrequency Raman spectroscopy was performed followed by optical absorption studies before and after the purification treatments, as well photoluminescence analysis has been done to assign the semiconducting chiralities. This analysis has allowed us to understand the changes in the tubes' morphology and physical properties. To the best of our knowledge, this study provides the first relevant results regarding the scalability of this purification process over a B-doped SWCNT keeping the most species on the resultant material and has become a significant step toward the chirality sorting.

PW10

57Fe Mössbauer study of iron phases in TiO₂ production

Michael Reissner (1)

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TiO₂ white pigment [1] has found important applications in catalysis, printing inks, plastics, papers, solar cells and pharmaceuticals. In the manufacture of TiO₂ pigments two technologies are used. Ilmenite ore is used in the production of TiO₂ pigment by sulphate process, whereas rutile ore is used in the production of TiO₂ pigment by chloride process. In the present work the possibilities of Mössbauer spectroscopy in analysis of Fe-bearing phases which appear in the manufacture of TiO₂ pigment by sulphate process will be shown and discussed. XRD, FE-SEM/EDS and magnetometry were also used as supporting techniques. Ilmenite ore from Australia used in the manufacture of TiO₂ pigment (Cinkarna, Celje, Slovenia) is analyzed. In this technology it is very important to know the Fe²⁺/Fe³⁺ ratio in ilmenite ore [2,3]. Generally, ilmenite can be associated with other minerals, such as hematite, magnetite, rutile, fayalite, zircon, quartz and various aluminosilicates [1]. Mössbauer spectra of ilmenite ore were recorded from RT to liquid He temperature. The changes in the Mössbauer spectra, as

well as corresponding magnetometric measurements are discussed. In the manufacture of TiO₂ by sulphate process a significant amount of copperas (FeSO₄·7H₂O) crystallizes as a by-product. In the technology mentioned copperas is calcined with the aim to produce H₂SO₄ acid which is returning to the process of ilmenite ore digestion. The RT Mössbauer spectrum of calcined copperas showed the superposition of one sextet corresponding to hematite and one central quadrupole doublet of small relative intensity. However, the Mössbauer spectrum of the magnetic fraction separated from calcined copperas with permanent magnet also showed the presence of substoichiometric magnetite (Fe_{3-x}O₄). Sulphur detected by EDS analysis of calcined copperas was a result of incomplete oxidation of copperas. Copperas produced as a by-product undergoes oxidation at ambient conditions and this can be also monitored by Mössbauer spectroscopy. Copperas can be utilized in the manufacture of yellow pigment (α-FeOOH) with the aim to optimize the cost of TiO₂ pigment production.

- [1] G. Auer, Titanium dioxide, in Industrial inorganic pigments (Eds.: G. Buxbalm, G. Pfaff), Wiley- VCH, Weinheim (2005), pp. 51-81
 [2] D. Jancik, M. Mashlan, R. Zboril, J. Adetunji, K. Nomura, Czechoslovak, J. Phys. 55 (2005) 803-811.
 [3] B. Saensunon, G.A. Stewart, R. Pax, Int. J. Miner. Process. 86 (2008) 26-32

PW11

Crackling noise and avalanches in porous media under compression

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This study investigates the behavior of nanoporous media under compression. Some porous materials respond to the application of an external force in a sequence of jerky events due to the correlated collapsing of nanometer-scaled pores. Jerks often combine to produce crackling noise. Such nano-structural movements form avalanches where each

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jerk triggers others and the behavior of the system can be described by a power-law distribution. Therefore, the avalanches appear in broad size distributions and show scale-invariance. It has been discovered that such jerky events are independent of both the macroscopic and microscopic details of the systems [1] and, therefore, the critical exponents of such power-laws are universal.

The measurement technique involves an analysis of strain drops with a Diamond DMA (Dynamical Mechanical Analyzer, PerkinElmer) at slowly varying compressive stress (0.1 mN/s - 10mN/s). The samples selected were on the one hand Gelsil and Vycor, both SiO_2 -based synthetic materials, which have been studied previously with acoustic emission and, on the other hand, Shale which is a natural porous sedimentary rock. The jerky evolution of the sample's height with time is analyzed in order to determine the corresponding power-law exponents for the maximum velocity distribution, the squared maximum velocity distribution as well as the aftershock activity in the region before macroscopic failure.

A comparison with recent results from acoustic emission data on the same materials [2] shows similitude in the statistics, although the two methods operate on different spatial and temporal scales. Moreover, the obtained power-law exponents are in reasonable agreement with theoretical mean-field values [3].

[1] J. P. Sethna, K. Dahmen and C. R. Myers: Crackling noise. *Nature*. 2001; 410 (6825): 242-250

[2] J. Baró, Á Corral, X. Illa, A. Planes, E.K.H. Salje, W. Schranz, D.E. Soto-Parra, and E. Vives: Statistical similarity between the compression of a porous material and earthquakes. *Phys. Rev. Lett.* 2013; 110: 088702

[3] M. LeBlanc, L. Angheluta, K. Dahmen, N. Goldenfeld: Universal fluctuations and extreme statistics of avalanches near the depinning transition. *Phys. Rev. B.* 2013; 87:022126

PW12

Failure Detection in Commercial Thermoelectric Modules using Infrared Thermography

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In this work we present a method to detect failures in commercial thermoelectric (TE) modules using Infrared (IR) thermography. The TE modules consist of 252 pn thermoelectric junctions based on Bi_2Te_3 alloys. The dimension of a TE module is 40 mm x 40 mm x 4,7 mm. In general, failures which are located inside the TE module (typically cracks, physical damage, destroyed soldering by electrical overload) can not be detected optically. Therefore, to detect such failures IR Thermography is a practicable (non destructive) measurement technique that generates a high resolution two-dimensional temperature map [1, 2]. For this, the TE module is placed with one side on an aluminum heat sink (held at RT) with an additional thin layer of thermal grease to obtain a good thermal contact. The other side (front side) is heated up by electrically sourcing and is exposed to ambient natural convection. The front side was inspected by the IR camera which is a cooled 320 x 256 pixel FPA with a thermal resolution of 20 mK and is sensitive in the spectral range of 3-5 microns. A frame rate of 50 Hz was chosen and the spatial resolution was 5.75 pixel/mm.

Due to the fact that a failure behaves like an increased electrical resistance it appears on the IR image in the form of a hotspot. Therefore, for internal energy generation by Joule heating the TE module can electrically be sourced either with AC or DC voltage. In general, the TE module was electrically sourced with a DC voltage of 6.1 V and a current of 1.3 A. Hotspots were detected at the surface of the TE module which indicates failures at these locations. To get information about the nature of the failure a three-dimensional cone-beam X-ray computed tomography (XCT) was carried out. In most cases the nature of the failures were mainly cracks in the legs of the TE module. Alternatively by applying an AC voltage one can carry out Lock In Thermography and by analyzing the phase images one can get information about the depth of the failure.

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Additionally, simulations of the temperature rise on the surface of a TE module were carried by finite element method under DC conditions. The failures were modeled by an increased electrical resistance of a leg compared to a "good" leg.

[1] D.P. Almond and P. M. Patel, *Photothermal Science and Techniques* (Chapman & Hall, 1996).

[2] G. Hendorfer, *Materials Testing* 51, 405-411 (2009).

PW13

Study of atomic motion in rubidium borate glasses

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Atomic Scale X-ray Photon Correlation Spectroscopy (aXPCS) utilizes coherent X-rays to probe the dynamics of materials on an atomic scale. It was used with great success to study atomic diffusion in crystals [1], but its application was recently extended to glasses as well [2]. Rubidium borate glasses serve as an example for fast ion-conducting alkali borate glasses and are a promising candidate for future applications in energy storage as well as in many other fields. In this work the ionic motion in rubidium borate glasses was studied via the aXPCS method.

Correct data analysis of an aXPCS measurement of amorphous materials requires the knowledge of the partial structure function of the diffusing atomic species, i.e. in this case the alkali ions. We used the pair distribution function (PDF) method to investigate the structure of rubidium borate glasses and Metropolis Monte Carlo simulation to extract the required partial structure factor. The parameters of a Born-Mayer-Huggins potential used by Verhoef and den Hartog [3] for structural simulations of alkali borate glasses were modified to fit the experimental scattering data.

This work was financially supported by the Austrian Science Fund (FWF) P28232.

- [1] M. Leitner, B. Sepiol, L.-M. Stadler, S. Pfau and G. Vogl, *Nat. Mater.*, 8, 717 (2009)
- [2] M. Ross, M. Stana, M. Leitner and B. Sepiol, *New J. Phys.*, 16, 093042 (2014)
- [3] A.H. Verhoef and H.W. den Hartog, *J. Non-Cryst. Solids*, 182, 235 (1995)

PW14

Studying the effect of dispersion corrections in ab initio water using neural network potentials

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In computational materials science the choice of an appropriate potential energy model is crucial to accurately predict the properties of materials. While sophisticated ab initio methods can be used to calculate energies and forces with high accuracy, their considerable computational cost limits their application to relatively small systems and makes large-scale molecular dynamics (MD) simulations impossible in most cases. Empirical potentials, on the other hand, are computationally far less demanding but also lack in accuracy, particularly if covalent bonds are broken or formed. An alternative approach put forward recently consists in training artificial neural networks (NN) to predict the energies and forces [1]. This new method provides the accuracy of first-principles calculations at a fraction of their computational cost. Here, we present neural network potentials for bulk water and ice based on RPBE and BLYP ab initio reference data and study the effect of dispersion corrections (D3) as proposed by Grimme et al [2]. From interface pinning simulations [3] of large systems we show that van der Waals corrections are essential to reproduce reasonable melting temperatures as well as water and ice densities. In addition we present our efforts to compute the temperature of maximum density (TMD) line for the RPBE-D3 and BLYP-D3 model at high negative pressures.

- [1] Behler, J., and Parrinello M., Phys. Rev. Lett. 98, 146401 (2007).
- [2] Grimme, S. et al., J. Chem. Phys. 132, 154104 (2010).
- [3] Pedersen, U. R., J. Chem. Phys. 139, 104102 (2013).

PW15

Plasmon dispersion and lifetime in dilute two-dimensional electron systems

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Many systems relevant for technological applications are well modeled by interacting electrons confined to two dimensions (2D): Notable examples are metallic monolayers on insulating substrates, semiconductor hetero-structures and inversion layers. Many-body effects due to spin-polarization and, especially, correlations among the electrons, result in a deviation from the predictions based on the Random Phase Approximation (RPA). Correlation effects are considerably more pronounced in 2D than in the bulk, in particular for low densities. We present a detailed study of the plasmon properties for cases where the failure of the RPA and similar approaches is significant. For the conventional („charge“) plasmon, the emphasis lies on the life-time arising from two-pair fluctuations included the dynamic pair theory [1]. We study the dependence on density and wave vector and critically compare the results with those from other approaches. Finally, we present preliminary results on the spin-plasmon occurring only in polarized systems [2].

- [1] H. M. Böhm, R. Holler, E. Krotscheck, and M. Panholzer, Phys. Rev. B 82, 224505, 2010
- [2] D. Kreil, R. Hobbiger, J. T. Drachta, and H. M. Böhm, Phys. Rev. B 92, 205426, 2015

PW32

Towards a pump-probe x-ray scattering setup at the Austrian SAXS beamline

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Through the advent of free electron lasers as well as ultrafast lab-based laser systems, highly time resolved methods have risen to be essential tools to study the interaction between light and condensed matter. [1] However, both of the named techniques lack the ability to directly track structural changes on the atomic scale, immediately after irradiation. The pulsed nature of synchrotron light, on the other hand, opens up a window at exactly these time- and length-scales: filming sub-nanometer structural changes of liquid- and solid-state systems with picosecond time resolution.[2]

We are implementing such an optical-pump hard-x-ray-probe setup at the Austrian SAXS beamline at the Elettra. A custom radio-frequency circuit that is in phase with the storage ring cavity synchronizes all necessary devices and delivers the gating pulses required for x-ray bunch discrimination at the detector. Further, a femtosecond laser will be installed to deliver high-power pulses in the VIS-IR range to initiate light-induced phenomena in liquid and solid samples. We will present the detailed setup with its specifications and provide an overview of the current challenges we are facing.

[1] B. W. J. McNeil, N. R. Thompson, *Nature Photonics* 4, 2010, 814-821.

[2] K. Jeongho, K. H. Kyung, H. Ihee, *Chemical Communications* 52, 3734-3749.

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PW16

Two-Dimensional Iron Tungstate Honeycomb Layers on Pt (111)

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The exceptional physical properties of graphene have sparked tremendous interests toward two-dimensional (2D) materials with honeycomb structure. We report here the successful fabrication of 2D iron tungstate (FeWO_x) layers with honeycomb geometry on a Pt (111) surface, using the solid-state reaction of $(\text{WO}_3)_3$ clusters with a FeO (111) monolayer on Pt (111). The formation process and the atomic structure of two commensurate FeWO_x phases, with (2×2) and (6×6) periodicities, have been characterized experimentally by combination of scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and temperature-programmed desorption (TPD) and understood theoretically by density functional theory (DFT) modeling. The thermodynamically most stable (2×2) phase has a formal FeWO_3 stoichiometry and corresponds to a buckled $\text{Fe}^{2+}/\text{W}^{4+}$ layer arranged in a honeycomb lattice, terminated by oxygen atoms in Fe-W bridging positions. This 2D FeWO_3 layer has a novel structure and stoichiometry and has no analogues to known bulk iron tungstate phases. It is theoretically predicted to exhibit a ferromagnetic electronic ground state with a Curie temperature of 95 K, as opposed to the antiferromagnetic behavior of bulk FeWO_4 materials.

PW17

Study of inter-diffusion and its effect on the magnetization coupling in Fe/MgO/Fe/MgO/GaAs (001) heterostructure

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Intermixing at the interface between spin-polarized ferromagnetic layers and semiconductor templates is expected to significantly reduce the spin injection efficiency of spin and magnetoelectronics devices and recommends the use of appropriate diffusion as well as tunnel barriers. Here we report on the growth of epitaxial Fe/MgO/Fe tunnel magneto-resistive (TMR) device on GaAs (001) and study the effect of interdiffusion on the magnetization coupling between the ferromagnetic layers of the device. We present in-situ stress measurement of each layer during its growth that would provide direct information on the strain relaxation due to interdiffusion. Thereafter, we present the magnetization results of the TMR structure with varying MgO (diffusion/tunnel) barrier thickness.

PW18

Monodisperse tungsten oxide cluster deposition from solution

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Perfectly monodisperse clusters of oxides are critically important model systems for catalysis studies because they allow the rigorous analysis of reaction mechanisms, and variations at the single-atom level can already be reflected in their reactivity. The generation and intact immobilisation on a suitable substrate of such clusters is quite challenging, and usually requires mass spectrometric size selection and

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sophisticated soft landing protocols to make such studies successful. Tungsten (VI) oxide in particular holds promise as a visible-light photocatalyst, but is quite reactive and can be challenging to immobilise in a well-defined manner in vacuum [1].

Here, we present a solution-based protocol for the preparation of monodisperse cyclic tris (tungsten (VI) trioxide) clusters, $(\text{WO}_3)_3$. The clusters can be harvested efficiently on the boron nitride nanomesh [2], an atomically thin layer of hexagonal boron nitride on Rh (111) with strong corrugation, and a promising platform for self-assembly [3] and electrochemical functionality [4]. The triangular $(\text{WO}_3)_3$ clusters adsorb in the 'pores' of the nanomesh, where they were imaged with submolecular resolution using electrochemical scanning tunnelling microscopy. The decorated surface was transferred to vacuum where the chemical identity of the clusters was confirmed with XPS. To our knowledge, this is the first successful example of self-assembly on the nanomesh from solution. We expect that proper control over deposition conditions will allow tuning of the number of clusters per pore, making this a promising model system for on-surface catalysis studies.

We contrast this finding with deposition of the same source material on rutile TiO_2 (110) in liquid, on which the clusters appear to react and form chains, akin to some observations of sublimated WO_3 in vacuum [5]. Even though the clusters are likely hydroxylated in aqueous solution, this behaviour indicates surprising parallels with UHV and suggests that, in many cases, solution-based procedures complement vacuum methods.

1. Li, S.-C., et al., Preparation, Characterization, and Catalytic Properties of Tungsten Trioxide Cyclic Trimers on FeO (111) /Pt (111). *J. Phys. Chem. C*, 2012. 116: p. 908-916.
2. Corso, M., et al., Boron nitride nanomesh. *Science*, 2004. 303: p. 217-20.
3. Berner, S., et al., Boron nitride nanomesh: functionality from a corrugated monolayer. *Angew. Chem. Int. Ed.*, 2007. 46: p. 5115-5119.
4. Mertens, S.F.L., et al., Switching stiction and adhesion of a liquid on a solid. *Nature*, 2016. in press. (DOI: 10.1038/nature18275)
5. Wagner, M., et al., Structure and Bonding of Tungsten Oxide Clusters on Nanostructured Cu-O Surfaces. *J. Phys. Chem. C*, 2011. 115: p. 23480-23487.

PW19

Fouling of heat exchanger surfaces caused by double salt formation

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In the industrial process of pulping one faces problems with formation of deposits on the heat exchanger of evaporators. To tackle this issue one has to think about crystallization and the beginning of the nucleation process [1]. The state of the art for hindering this problem is to start a heterogeneous nucleation on germs (precipitator ash particles) which are put into the liquid with a solids content of more than 55%. Thus, the nucleation of Burkeite and Na_2SO_4 starts in the concentrated liquor. The crystallization starts preferably on the nucleation germs in the liquor and is not available for nucleation on the heat lamella. Beside Burkeite and Na_2SO_4 crystals, there are other double salts in the liquor which are not crystallizing on these existing nuclei provided by the ash particles. Here, center of nucleation of the Di-Carbonate starts from the metal surface which results in deposits on the heat lamella and thus decreases the heat exchange. We tried to use available process related compounds with high boiling point to cover the metal surface. With several different compounds tested we came to the conclusion that for our process organic soaps and homologue compounds worked best. They protect the metal surface and suppress the formation of new crystallization germs for the buildup of larger deposits. This results in less frequent washing cycles and increased evaporation capacity.

[1] D.Freyer and W.Voigt, Monatshefte für Chemie 134 (2003) 693-719

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PW20

Epitaxy of Highly Ordered Conjugated Organic Semiconductors Supported by Hexagonal Boron NitrideJakob Alexander Genser (1)

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We examine hexagonal boron nitride (hBN) as a van der Waals dielectric substrate for epitaxial growth of highly ordered networks of organic semiconductor crystallites. For this purpose, we use para-hexaphenyl ($C_{36}H_{26}$, 6P), a rod-like conjugated molecule. Thin-films of 6P were deposited by hot wall epitaxy onto SiO_2/Si supported exfoliated hBN flakes. We demonstrate how the number of layers of the supporting hBN and growth parameters affects the morphology of the 6P crystallites. Furthermore, we investigate how the rotational symmetry of the hBN substrate is reflected by the growth directions of the 6P needle-like crystallites. The observed three-fold ordering of the needle-like crystallites is in the agreement with the preferential adsorption sites of 6P on hBN, obtained by ab-initio calculations. The results show that by tuning the growth parameters several tens of micrometers long, and well oriented needle-like crystallite networks can be obtained on multi-layer hBN support.

PW21

Crystal Morphology Investigation of LiFePO₄ Microparticles using AFM and First-Principles CalculationsKevin-Peter Gradwohl (1)

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Olivine structure LiFePO_4 (LFP) is one of the most promising candidates for cathode materials in large scale applications. We investigated the geometry of faceted LFP microparticles by atomic force microscopy (AFM). Different particle shapes were obtained by changing the precursor concentration and introducing surfactants in a modified hydrothermal synthesis process proposed by Ref. [1]. With the quantitative AFM surface information (edge angles and facet tilts) we were able to determine the Miller indices of each facet by an error minimization technique. The facet orientations have been compared to previous first-principles studies [2]. All facets observed were low surface energy facets according to Ref. [2] except for (210) which was not considered there. We calculated the surface energy of (210) within density functional theory in the generalized gradient approximation (GGA) + U framework and found that the missing facet contributes about 2.5% to the total area of the Wulff-Plot.

[1] X. Qin, J. Wang, J. Xie, F. Li, L. Wen, X. Wang, *Phys. Chem. Chem. Phys.*, 2012, 14, 2669

[2] L. Wang, F. Zhou, Y. S. Meng, G. Ceder, *Phys. Rev. B*, 2007, 76, 165435

PW22

Metastable Behavior of Thin-Film Solar Cells under Colored Light

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Thin film solar cells based on an absorber made of copper, indium, gallium, selenium and sulfur (also called CIGS or chalcogenides) are a promising alternative to conventional solar cells. CIGS solar cells have reached efficiencies of above 21% and prices below 1\$/W. However, they have the main disadvantage to show electric metastable behavior. While the metastable processes in all materials of CIGS solar cells are well known on a microscopic level, their influence on macroscopic parameters like open circuit voltage, maximum power point and short

circuit current are hardly known. Thereby it is impossible to accurately power rate CIGS solar cells. In order to improve their impact on the global PV market, research on this topic needs to be done.

This work focuses on metastable effect of CIGS solar cells where the cell's macroscopic parameters – especially V_{OC} , FF and P_{MPP} – change due to illumination. It can take up to several hours to reach a saturated state and cells completely relax to the initial state when stored in the dark. It is known that the amount as well as the direction (decrease/ increase) of the illumination effect depend not only on the materials used, their quality and the working point of the solar cell, but as well on the wavelength of the incident light. Especially the so called “blue light effect” and the so called “red light effect” can be found in the literature. This work tries to get deeper insights into these two effects by performing illumination measurements under differently colored light. That measurements have been performed for CIGS solar cells of different performance quality (efficiencies from 9.4% to 13.4%) and two different buffer layers (CdS and ZnO), in order to gain information on the interaction between intrinsic characteristics of the samples and the irradiance spectra.

One of the main findings of this work was that the metastable effects on macroscopic level show smooth transitions from low to high quality of the cells as well as from low to high wavelength. Furthermore the effects of the low quality solar cells are similar for both buffer layer materials but are different for high quality cells, which is directly related to the defect structure. The changes in V_{OC} and P_{MPP} have reached up to +20% in some specimen.

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PW23

The effect of anharmonic vibrations in electronic transitions on time-dependent spectroscopic signals

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Emission spectrum of an electronic transition, modulated by a set of harmonic vibrations, is a mirror image of the absorption spectrum of the same system [1]. In most experimental cases however, this symmetry is broken. We describe this effect by lifting the restriction of the commonly used displaced harmonic oscillator approach. Instead we employ displaced anharmonic potential surfaces coupled to a harmonic bath to describe an electronic two-level system with vibrational features. The anharmonicity of the potential surfaces is taken into account by adding a cubic term to the potential energy. Asymmetry between absorption and emission spectra of a molecule is then a witness to the system's anharmonicity. Going beyond the characterization of linear spectra, we show the effect of anharmonicity on time-dependent non-linear spectroscopic signals. With such a displaced anharmonic oscillator system, we are able to explain the lack of certain vibrational signals in multi-dimensional nonlinear spectra. This effect observed in several experimental studies is beyond the purely harmonic oscillator model [2].

[1] G. Herzberg, *Molecular Spectra and Molecular Structure III (Polyatomic Molecules)*, D. Van Nostrand 1966

[2] T. Mancal et al. System-Dependent Signatures of Electronic and Vibrational Coherences in Electronic Two-Dimensional Spectra, *The Journal of Physical Chemistry Letters*, 3 (11), 1497-1502, 2012

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PW24

Outcoupling as a tool to perform multiple measurements on a Bose-Einstein condensate

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We propose to use outcoupling as a tool to study the quantum measurement back-action on a Bose-Einstein condensate (BEC). On our atomchip based cold atom experiment BECs are magnetically trapped and typically imaged after some time of flight. Manipulating the internal state of a fraction of atoms in the magnetically trapped BEC such that they leave the trap allows to probe the same cloud of ultracold atoms more than once or to perform successive measurements on small parts of the system. Here we discuss possible applications and existing challenges of such a measurement scheme.

PW25

Chip Integrated Nano-Fiber Atom-Photon Interface

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Micro-Optics on Atom chips;

The experiment concerns the combination of two established concepts in Ultracold-Atom physics. The first is trapping atoms magnetically on atom-chips in a one dimensional fashion. The second is using nano-fiber based elongated cavities which are integrated close to the chip. Together, this constitutes a unique platform to probe atom-photon interactions. The intrinsically mode-matched resonator consists of two fiber Bragg gratings (FBG) that are being lased onto the fiber.

Data shows that an atomic ensemble couples strong to the cavity in a collective way, applying the common definition of 'strong coupling', data shows that the atomic ensemble couples in such a way to it.

Furthermore I will present most recently taken measurement where we

collect the light that the excited atoms send into the cavity, i.e. fluorescence spectrum. A few exemplary applications for our system are:
 Self-organization of atoms due to Bragg Scattering into the cavity mode;
 Frequency selective fluorescence spectroscopy of atoms in the surface-induced potential of the fibre;
 Strong nonlinear interactions between individual photons;
 Realizing a Photon-Transistor

PW26

Gyrofluid impurity transport modelling for tokamaks

Eduard Reiter

Markus Held, Alexander Kendl, Matthias Wiesenberger

Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, AUT

A magnetically confined thermonuclear fusion plasma typically consists of the main hydrogen isotopes, stripped electrons and fusion products. Besides that, in tokamak experiments energetic particles inevitably leave the plasma volume, erode plasma-facing materials and hence result in impurities - a multitude of neutral and ionized atoms and molecules, which penetrate deeply into and severely pollute the plasma [1].

Radial transport of charged particles and hence of ionized impurities is dominated by turbulent convection, driven by gradients in pressure, density or the magnetic field present in a toroidal fusion plasma [2]. The full-F FELTOR code, currently developed in our group at Innsbruck University, provides numerical gyrofluid modelling [3]. Results are self-consistent even in the vicinity of the scrape-off layer, where field-aligned turbulent structures ('blobs') of perturbation amplitudes comparable to the magnitude of background profiles emerge. Furthermore energy conservation as well as consistent treatment of the ion temperature is inherent to the model.

An extension of the FELTOR framework to account for multiple ion-species and hence for the evolution and back-reaction of impurities is presented. We demonstrate studies of the center of mass velocity and impurity dynamics for the propagation of blobs in a restricted model for a simplified 2-d geometry.

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- [1] C. Angioni et al., Phys. Plasmas 2007, 14, 055905.
[2] G. R. Tynan et al., Plasma Phys. Control. Fusion 2009, 51, 113001.
[3] M. Wiesenberger et al., Phys. Plasmas 2014, 21, 092301.

PW27**Permanent molecular dipole moments in quantum diffraction**Christian Knobloch (1)

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Diffraction of molecules is a clear evidence for the quantum wave nature of delocalized matter. While coherent interactions like the attractive Casimir-Polder force lead to high contrast diffraction patterns, non-coherent interactions induce decoherence and dephasing. In this context we study the diffraction pattern of polarizable and polar molecules after passing a nano-mechanical mask. We observe that the diffraction patterns of molecules with a permanent electric dipole moment have a significantly reduced contrast compared to those of non-polar molecules. The strength of this effect depends on the material of the grating and points towards an interaction between charges in the material and the permanent dipole moment of the molecule. This is in agreement with a theoretical analysis which states that the dipole moment in combination with the molecular rotation leads to a phase-shift which depends on the orientation and the internal state of the molecule. This leads to an effective dephasing of the matter-wave and is of relevance for future matter wave experiments with highly polar biomolecules.

PW28

Bright Solid State Source of Photon Triplets

Max Prilmüller (1)

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Producing advanced quantum states of light is a priority in quantum information technologies. While remarkable progress has been made on single photons and photon pairs, multipartite correlated photon states are usually produced in purely optical systems by postselection 1–3 or cascading 4, with extremely low efficiency and exponentially poor scaling. Multipartite states enable improved tests of the foundations of quantum mechanics as well as implementations of complex quantum optical networks and protocols 3. It would be favorable to directly generate these states using solid state systems, for better scaling, simpler handling, and the promise of reversible transfer of quantum information between stationary and flying qubits. Here we use the ground states of two optically active coupled quantum dots to directly produce photon triplets. The wavefunctions of photogenerated excitons localized in these ground states are correlated via molecular hybridization and Coulomb interactions. The formation of a triexciton leads to a triple cascade recombination and sequential emission of three photons with strong correlations. The quantum dot molecule is embedded in an epitaxially grown nanowire engineered for single-mode waveguiding and improved extraction efficiency at the emission wavelength. We record 65.62 photon triplets per minute, surpassing rates of all earlier reported sources 4, in spite of the moderate efficiency of our detectors. Our structure and data represent a breakthrough towards implementing multipartite photon entanglement and multi-qubit readout schemes in solid state devices, suitable for integrated quantum information processing.

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1. Bayer, M. et al. Coupling and entangling of quantum states in quantum dot molecules. *Science* 291, 451–453 (2001).
2. Vurgaftman, I. Meyer, J. R. & Ram-Mohan, L. R. Band parameters for III–V compound semiconductors and their alloys. *J. Appl. Phys.* 89, 5815 (2001).
3. Zanolli, Z. Fuchs, F. Furthmüller, J. von Barth, U. & Bechstedt, F. Model GW band structure of InAs and GaAs in the wurtzite phase. *Phys. Rev. B* 75, 245121 (2007).
4. Govorov, A. O. Spin and energy transfer in nanocrystals without tunneling. *Phys. Rev. B* 68, 075315 (2003).

PW29

Hybrid approach to high-pressure gas discharge simulation

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As is known direct solution of Boltzmann kinetic equation is of great interest for theoretical investigation of various gas discharges. Such approach gives the most important information on discharge formation and evolution due to providing electrons and ions distributions functions at given time point. Unfortunately, complete numerical solution of Boltzmann equation for multi-component gas discharge plasma is a challenge even for one-dimensional problems. That is why usually gas discharges are described in terms of moment models with drift-diffusion approximation or by using particle-in-cell simulations with Monte-Carlo collisions. Main disadvantage of these simplified techniques is that the description of fast particles (e.g. runaway electrons) is substantially unfeasible, especially for high pressures and strong overvoltages. Here we present the theoretical approach for discharge simulation in dense gases based on a hybrid approach. Within the framework of hybrid mathematical model, plasma hydrodynamics and kinetics are both used describing the dynamics of different components of low-temperature discharge plasma. As an example, we apply our investigation approach to coaxial relativistic gas diode. Namely, it was shown that electrons power spectrum of the discharge contains group of electrons

with the so-called „anomalous“ energies (above maximal applied voltage value) that was not correctly predicted before. Comparison of our calculation results with the existent experimental data gives a good agreement for major process parameters.

PW30

How does hydrogenation influence the backbone stability of pyrene?

Michael Wolf (1)

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Both polycyclic aromatic hydrocarbons (PAHs) and their hydrogenated counterparts are thought to be present in the interstellar medium [1,2]. Hydrogenation may protect PAHs by allowing for internal cooling through evaporation of the additional H atoms. Such a protective effect was indicated in core-electron excitation experiments by soft x-rays of hydrogenated coronene cations ($C_{24}H_{12+m+}$; $m = 0-7$), where the hydrogenated molecules lost fewer of their native H atoms than native coronene ($m = 0$) [3]. However, the carbon backbone is also weakened by the conversion of sp^2 -type aromatic bonds to sp^3 -type aliphatic bonds. In this work we present two types of experiments with native and hydrogenated pyrene cations ($C_{16}H_{10+m+}$; $m = 0, 6, \text{ or } 16$). In collision induced dissociation experiments, performed at Stockholm University, keV pyrene ions collide with a stationary He target resulting in center-of-mass collision energies in the range of 20–200 eV. We find that the absolute carbon backbone fragmentation cross section increases as we increase the degree of hydrogenation [4]. We also find that CH_x -loss, which only proceeds through prompt knockout for native pyrene, is mainly a statistical process for hydrogenated pyrene [5]. In photo induced dissociation experiments, conducted at the electrostatic ion storage ring ELISA [6] at Aarhus University, 22 keV pyrene ion bunches were overlapped with a 5 ns laser pulse with a wavelength between 420–455 nm [7]. In these experiments we can deduce the number

of photons absorbed before fragmentation proceeds by measuring the fragment yield as a function of laser pulse energy. This yield follows a power law, where the exponent gives the photon dependency for a given photon energy, E . From least square fits to the total fragmentation yields we conclude that $C_{16}H_{10+}$ must absorb three photons ($E = 2.72$ eV), $C_{16}H_{16+}$ must absorb two photons ($E = 2.88$ eV), and $C_{16}H_{26+}$ must absorb only one photon ($E = 2.95$ eV) of similar energy before carbon backbone fragmentation occurs [7].

These results show that carbon backbone fragmentation of pyrene (a small PAH) increases with the degree of hydrogenation. This is true for excitations in collisions with atoms as well as for excitations by photo-absorption. It remains to be investigated if larger PAHs would show the same behaviors when they are excited in similar ways.

- [1] A. G. G. M. Tielens, Rev. Mod. Phys., 85 1021 (2013).
- [2] J. D. Thrower, et al., Phys. Chem. Chem. Phys, 16 3381 (2014).
- [3] G. Reitsma, et al., Phys. Rev. Lett., 113 053002 (2014).
- [4] M. Gatchell, et al., Phys. Rev. A, 92 050702 (2015).
- [5] M. Wolf, et al., Eur. Phys. J. D, 70 85 (2016).
- [6] J. U. Andersen, et al., Rev. Sci. Instrum., 73 1284 (2002).
- [7] M. Wolf, et al., Astrophys. J. (submitted).

PW31

Fundamental aspects of particle transport in high power impulse magnetron sputtering plasmas

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High power impulse magnetron sputtering (HiPIMS) is a modern technique to produce thin films with superior quality. During high voltage pulses in the μs range power loads in the range of several MW/m² are achieved on the target. The resulting plasma has an ionization degree of up to 90% and especially at the end of the pulses, a very high metal content. One aspect of this discharges is the natural occurrence of

high energetic metal ions. These metal ions are held responsible why HiPIMS exceeds direct current magnetron sputtering in terms of coating quality. On the other hand HiPIMS suffers from a reduced efficiency which impedes the commercialization of this promising technique. One important aspect in HiPIMS research is therefore to clarify the physics of particle transport from the target to the substrate. Additionally to diffusion across the magnetic field in front of the target, fluctuations in the electric field and plasma density can contribute to anomalous transport. Especially, during HiPIMS at elevated power/current densities, symmetry breaks and self-organization in the plasma torus are observed. The former homogeneous plasma torus is then decomposed in localized traveling ionization zones which are commonly referred to as spokes. Electric fluctuations from these structures are measured by an array of twelve electrical probes. From these data the calculated dispersion relations are used to study the fundamental physical processes. Time and energy resolved mass spectrometer measurements show that high energetic metal ions are present if the plasma is in spoke mode. This suggests that an internal potential structure has to be present which accelerates ions which are born inside. Spokes are therefore not a peculiar aspect but the essence of HiPIMS plasmas!

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