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Faculty of Physics

Annual Report 2015 | 2016 | 2017

Faculty of Physics



**Faculty of Physics
University of Vienna
Annual Report
2015 | 2016 | 2017**

Message from the Dean



It is a pleasure and honor to present to you our 2015 – 2017 report. These three years were a period of remarkable growth in all parameters that indicate the success of an academic institution, such as the quality and quantity of scientific publications [1], the number of students on all levels [2], the number of excellence awards, and the amount of third-party funding [3]. I wish to thank all our 300 colleagues – scientists, administrative and technical personnel – who contributed to these achievements. The following pages will show many highlights of this period.

It is a particular delight to mention that Regina Hitzemberger, then group speaker of Aerosol Physics and Environmental Physics, became the Vice-Rector for Infrastructure in Oct. 2015. We are glad that Stefan Fredenhagen (Sept. 2016, *Mathematical Physics*) and Bernadett Weinzierl (Sept. 2017, *Aerosol and Cluster Physics*) followed our calls to a full professorship. Philip Walther (*Experimental Quantum Optics*) and Cesare Franchini (*Quantum Materials Modelling*) were promoted to a full professorship in Oct. 2017, and Ivette Fuentes (*Relativistic Quantum Information*) supported our faculty as a full professor on a three-year contract from Jan. 2015 to Dec. 2017 before she returned on a professorship in Nottingham.

Three new ERC Starting Grants were awarded to Bernadett Weinzierl, Toma Susi and Thomas Juffmann. An ERC Consolidator Grant went to Markus Aspelmeyer. Nikolai Kiesel won an FWF START Prize. Two highly competitive Special Research Programmes (SFBs) were extended: *Vienna Computational Materials Laboratory – ViCoM II* (speaker: Georg Kresse) and *Foundations and Applications of Quantum Science – FoQuS III* (deputy speaker: Anton Zeilinger).

We are proud of two newly established Christian Doppler Laboratories that are focused on *Mid-IR Spectrometry and Semiconductor Optics* (leader: Oliver Heckl) and on *Advanced Magnetic Sensing and Materials* (leader: Dieter Süss), respectively.

A new research platform, *TURIS – Testing quantum and gravity interface with single photons* (leader: Philip Walther), was founded, bridging physics and astronomy. The Erwin Schrödinger Institute was organizationally converted into a sustainable interdisciplinary research platform. Our faculty further participates in the *Environmental Sciences Research Network (ESRN)*.

30-40 new research projects contributed about 10 million euros per year to boosting our research activities and make the faculty an attractive employer for ambitious early-stage researchers.

This environment enables an excellent publication portfolio with about 320 peer-reviewed publications per year, many of them in prestigious journals and highly cited.

Markus Aspelmeyer, Georg Kresse and Jannik Meyer made it onto the *Highly Cited Researchers* list 2017, i.e. their papers ranked in the top 1% by citations for field and publication year in the *Web of Science*.

Our researchers represented our faculty with typically about 500 conference contributions per year.

The strong dynamics of a successful Faculty leaves us with a major challenge: a severe limitation of our premises. I therefore address my hope that an extension of high quality laboratory space as well as office space will become true within the next years.

To conclude, I would like to thank the rectorate for their continuous support in all of the above and also in the acquisition of major infrastructure items, for instance a costly new transmission electron microscope.

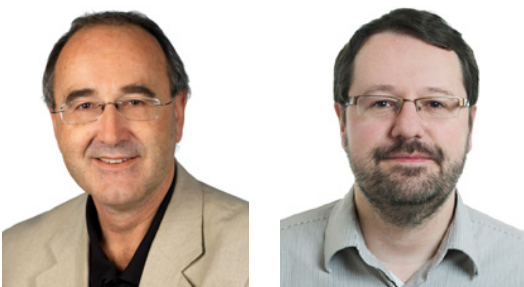
Univ.-Prof. Dipl.-Ing. Dr. Robin Golser
Dean, Faculty of Physics, 2014-2018

[1] See “Research Statistics”, p. 14.

[2] See “Students”, p. 14.

[3] See “Research Statistics”, p. 14.

Message from the Director of Studies



One of the most important developments of the previous academic years was the considerable increase in the number of students. The number of students who are enrolled and study actively at the Faculty of Physics increased from fewer than 1000 in 2009 to 1571 in 2015 and is now stabilizing at about 1600. Unfortunately, the teaching staff and the teaching hours did not increase likewise, which has the consequence that the ratio of teaching personnel to students decreased. Additionally, a lack of room, in particular large lecture halls, leads to full classes and laboratory courses, which are partly at or beyond the limit of capacity. On the other hand, the great personal commitment of the scientists ensures that we can still offer an excellent physics education for our students. We would like to thank everyone in the Faculty most sincerely for this.

In the period 2015-2017, the number of degrees increased also by nearly 50 per cent in comparison to the period before. A strong effort was the successful implementation of the new teacher's accreditation program, which has been finished now. Also, the old doctorate program expired and the students either finished their studies or were transferred into the new doctorate program.

One of the most challenging tasks was the development of a new curriculum for the bachelor and master of physics program. In intensive discussions, the Curricular Commission came to

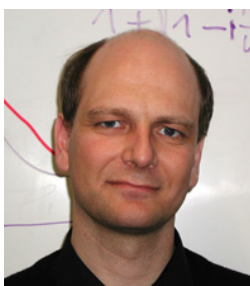
a conclusion, which was presented to the whole Faculty of Physics. In the next step, the Senate of the University of Vienna will discuss the proposal for the new curricula.

An excellent physics education, covering new teaching methods as well as including new research fields, is certainly one of the most important tasks of a university. We are looking forward to meeting this new challenge.

Univ.-Prof. Dr. Herwig Peterlik
Director of Studies 2016-2018

Univ.-Prof. Dr. Martin Hopf
Director of Studies 2014-2016

Message from the Vice-Director of Doctoral Studies in Natural and Technical Sciences representing Physics



Our doctoral students are the backbone of the scientific excellence of our Faculty. The high level of the achievements of these young researchers is crucial for our development and we are very proud of them. The newly established Vienna Doctoral School in Physics funded by the Vienna University Uni:docs excellence program has already welcomed a great portion of our graduate students and it provides a great example of who our human talents are. Additionally, a number of peer-reviewed topical doctoral programs funded by the FWF and the EU highlight the scientific excellence we have in house.

The research capacity and the excellence of our Faculty strongly rely on the currently 162 doctoral students, who are predominantly employed either as project/university assistants, or have personal grants. These students have a strong focus on research complemented by a small number of compulsory courses, which nevertheless encompass a broad spectrum of topical lectures and seminars as well as additional soft skill courses specially offered within our Doctoral Program. Furthermore, some of our courses have been specifically designed and devoted to the needs of the doctoral students, such as new seminars covering “Highlights of the Vienna Doctoral Students”. This has turned in the last years into the perfect scenario for our students to present and learn about new doctoral proposals and we have therefore combined this activity with the Faculty Open Presentation (FÖP). The implementation of the new Vienna Doctoral School in Physics (VDS-P) (led by Markus Arndt) in 2016 has allowed us to strengthen interactions across the research groups of all key research areas at the Faculty through joint scientific activities, lectures and networking events. Currently, the VDS-P has 38 doctoral students, including students hired via competitive international excellence programs.

We proudly host the research carried out by various senior faculty members, which has opened the possibility to incorporate students into several Internal Topical Programs (such as DCAFM and TURIS), and into the two

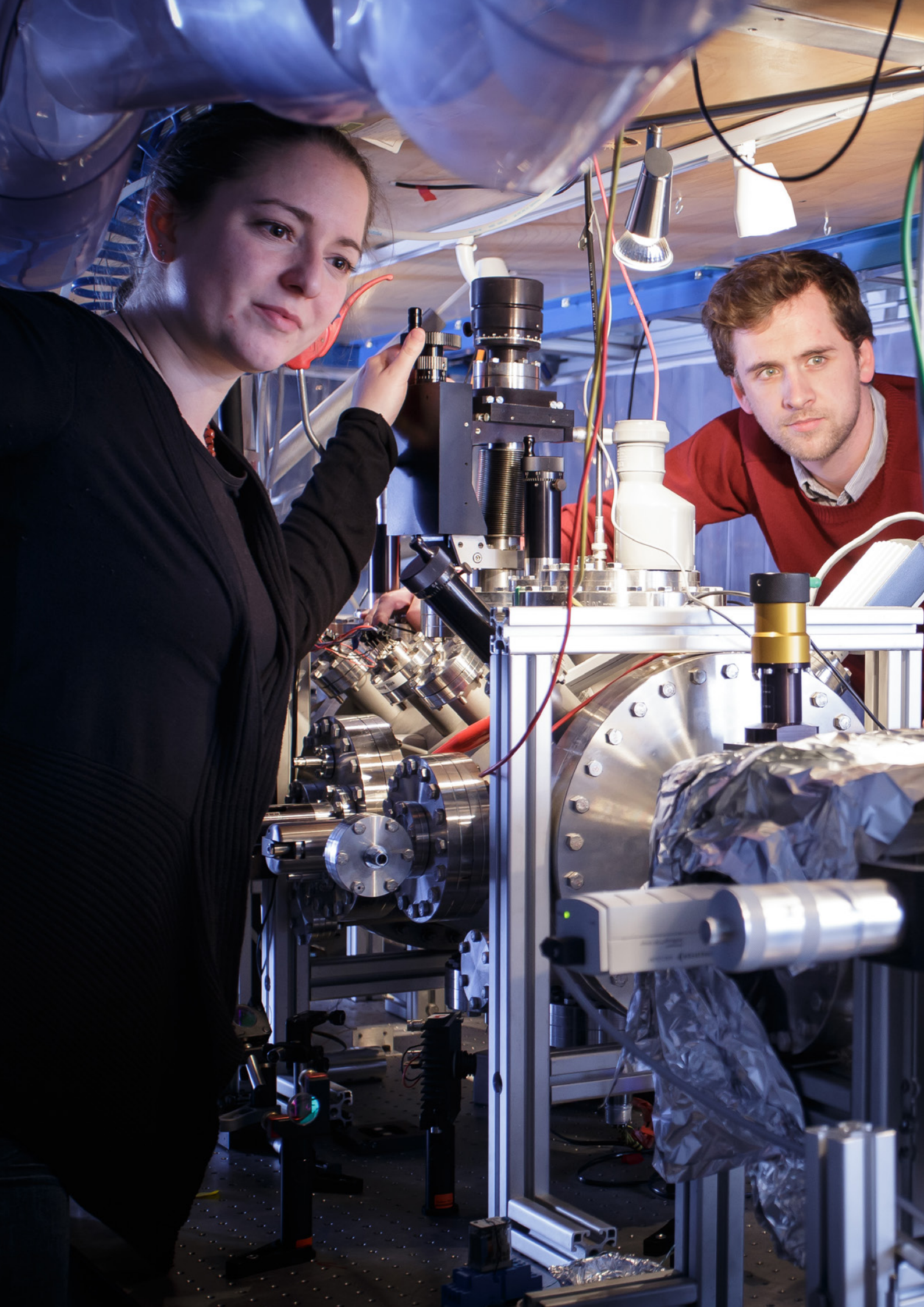
FWF-funded programs “Particles and Interactions” (co-speaker André Hoang) and “Complex Quantum Systems” (speaker Markus Aspelmeyer). The scientific staff currently supervising our doctoral students are partners or coordinators in four EU-funded International Training Networks (ITN). Among these, COLLDENSE, NANOTRANS, OMT and CLOUD-MOTION are currently running, and COMPLOIDS, PICQUE, cQOM and VERTIGO also took place during the 2015-2017 period. Not only international peer-reviewed programs have been our target but we have also put special emphasis on national initiatives. I am very delighted to have seen seven successful doctoral students to be admitted to the internationally reviewed excellence program Uni:docs of the University of Vienna between the years 2015 and 2017.


This is a sample of our work towards the excellence and visibility of our students. In summary, various milestones have been reached and I am particularly proud of results that can be considered emblematic. The VDS-P has clearly implemented a new structured research platform with coordinated and qualitative selection criteria, which, coupled to the FÖP twice a year, has remarkably reinforced the synergy of the Faculty’s collective strengths.

Univ.-Prof. Mag. Dr. Thomas Pichler
*Vice-Director of Doctoral Studies in Natural
and Technical Sciences, representing Physics
2014-2018*

Table of Contents

Faculty Facts and Figures	11
Research and Support Groups	17
Aerosol Physics and Environmental Physics	18
Basic Experimental Physics Training and University Didactics	26
Computational Materials Physics	30
Computational Physics	32
Dynamics of Condensed Systems	36
Electronic Properties of Materials	38
Faculty Center for Nano Structure Research	42
Gravitational Physics	44
Isotope Research and Nuclear Physics	47
Mathematical Physics	50
Particle Physics	52
Physics of Functional Materials	56
Physics of Nanostructured Materials	60
Quantum Optics, Quantum Nanophysics and Quantum Information	63
Workshop and Technical Services	69
News and Outreach	71
Christian Doppler Laboratory – “Advanced Magnetic Sensing and Materials”	72
Christian Doppler Laboratory for Semiconductor Optics and Mid-IR Spectroscopy	73
Research Platform TURIS	74
The Vienna Doctoral School in Physics (VDS-P)	75
Science Outreach	76





Faculty Facts and Figures

Faculty Facts and Figures

Structure of the Faculty

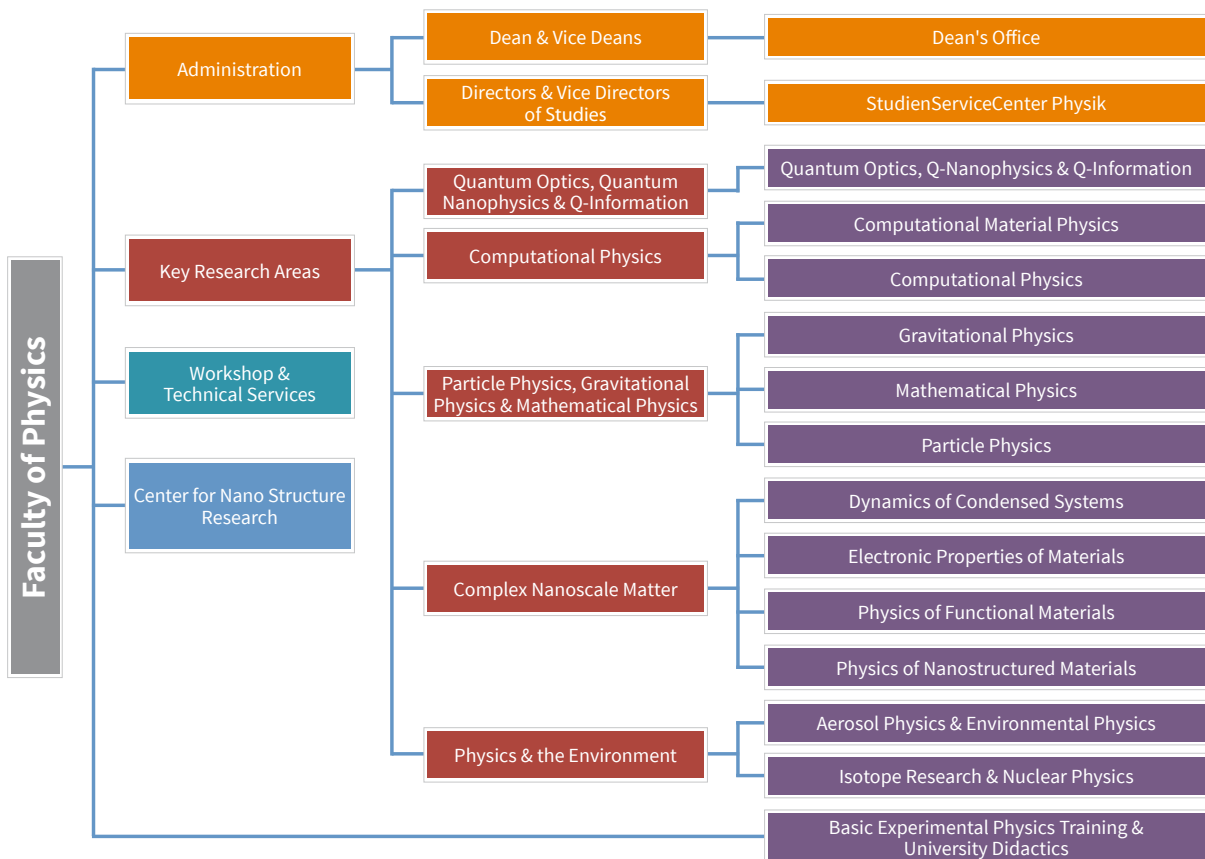
The Faculty is organized in 13 *Faculty Research Groups* (FRGs) that are active in 5 thematic *Key Research Areas* (KRAs), as shown in the organigram on the next page.

Each Faculty research group is organizational home for 1-7 *Individual Research Groups* (IRGs) and represented by a *FRG Group Speaker*.

Each IRG is the core unit for active research and currently unites 3-25 researchers, from Master student to full professor, in their passion for a particular focus in research.

An overview of the staff composition is shown below.

Scientific Staff (Heads)	2015	2016	2017
Professors	39	40	36
Visiting Professors	0	1	6
Senior Researchers	15	15	17
Senior Lecturers	3	5	6
Postdocs	76	83	90
Praedocs	118	114	126
Administrative and Technical Staff (full-time equivalents)			
University-funded	49	50	51
Third-party-funded	10	9	9
Total	59	59	60



Organizational Structure of the Faculty

Dean's Office

Throughout the entire reporting period 2015-2017, the Faculty of Physics was headed by the management team of Dean *Robin Golser* and Vice-Deans *Martin Fally* and *Philip Walther*.

As in previous years, *Gabriele Marzoner* held the position of director of the Dean's office, ensuring stability and continuity in our Faculty administration.

Director of Studies

Herwig Peterlik took over as Director of Studies from *Martin Hopf* in October 2016. Hopf continued to serve our students' needs as Vice-Director of Studies, along with co-Vice-Directors *Wolfgang Püschl* (until September 2016), *Helmut Rumpf* (until September 2016) and *Erhard Schafner* (from October 2016).

Director of Studies, Doctoral Program

Doctoral studies at the University of Vienna are organized across the borders of the Faculties. *Thomas Pichler* was Vice-Director of the Doctoral Studies Program in Natural and Technical Sciences, Research area Physics, throughout the entire reporting period.

In October 2016, the Vienna Doctoral School in Physics (VDS-P), a new structured doctoral program, was established, headed by *Markus Arndt*.

Scientific Advisory Board

The Scientific Advisory Board (SAB) of the Faculty of Physics consists of internationally renowned scientists who advise the faculty in scientific organizational and educational matters:

- Professor Emeritus Kurt Binder, Johannes Gutenberg University Mainz, Germany
- Professor Emeritus Detlev Buchholz, University of Göttingen, Germany
- Professor Eleanor Campbell, University of Edinburgh, UK
- Professor Elisabeth Giacobino, CNRS Paris, France

Research statistics

Research grants summary

- 2015: 26 new national, 9 new international grants, total third-party funding EUR 9.2 million
- 2016: 21 new national, 10 new international grants, total third-party funding EUR 7.7 million
- 2017: 34 new national, 15 new international grants, total third-party funding EUR 12.2 million

Publications in peer-review journals

- 2015: 307
- 2016: 302
- 2017: 341

Presentations at international conferences, national meetings and as part of seminar series and guest lectures

- 2015: 491
- 2016: 507
- 2017: 503

Students

Number of active students per semester	2015W	2016W	2017W
Bachelor, master, teacher accreditation	1572	1636	1611
PhD	144	153	167
Total	1715	1788	1776



Research and Support Groups



Aerosol Physics and Environmental Physics

Mission

The Aerosol Physics and Environmental Physics (AEP) Group at the Faculty of Physics of the University of Vienna combines highly sophisticated laboratory, ground-based and aircraft experiments with innovative modelling to study the fundamental physical and chemical properties of aerosol particles and clouds.

Current research focuses on related but different areas of aerosol science and covers the whole size spectrum from the nano- to the microscale. Topics investigated include nucleation phenomena, cluster physics, atmospheric and industrial nano-aerosols, aerosol optics, aerosol long-range transport, cloud physics, particle metrology, airborne aerosol measurements, radiative transfer in aerosol and cloud layers, and atmospheric aerosol dynamics and interactions.

The AEP group is dedicated to ground-breaking research in the field of aerosol science. The aerosol instrumentation developed and adapted by the AEP group stands at the forefront of ground-based and airborne measurement systems in the world.

The results achieved by the AEP group are important not only to promote a general understanding of physical problems related to aerosols, but also for addressing health- and technology-related questions, as well as societal challenges such as climate change.

Research Highlights

In the 2015-2017 period, several high-level research projects were carried out together with various international partners and research facilities. In March 2016, Univ.-Prof. Dr. Bernadett Weinzierl started her work as Professor for Aerosol and Cluster Physics at the University of Vienna. The research in the framework of two ERC Grants was continued, and a number of unique laboratory and field experiments were conducted. In the following, an overview of activities and research highlights of the AEP group is given.

Enhancement of measurement capabilities

In order to extend the measurement capabilities of the AEP group, new measurement systems were developed, adapted and characterized for ground-based and airborne applications. In addition, novel theoretical analysis methods were developed.

(1) A new second-generation *Cloud, Aerosol, and Precipitation Spectrometer* (CAPS) was optimized together with the manufacturer for airborne coarse mode aerosol and cloud measurements. The CAPS was extensively characterized, and a unique calibration method was developed. This allows for the first time high-precision calibrations of the CAPS over the entire size spectrum of the instrument between 0.5 and 930 μm not only under laboratory conditions, but also in the field. The CAPS was certified for airborne operation on the NASA DC-8 and the German Aerospace Center (DLR) Falcon research aircraft, and successfully deployed during four international aircraft field missions in 2016 and 2017 (Fig. 1).

(2) An integrated system for *Airborne High-resolution Extinction, Absorption and scattering Detection* (A-HEAD) was designed, built, tested and certified for airborne observations on the DLR Falcon research aircraft and successfully deployed during the A-LIFE field experiment (Fig. 2). A-HEAD consists of an Ecotech Aurora 4000 polar nephelometer (wavelengths: 450, 525 and 635 nm) which was adapted for airborne operation, two Brechtel Tricolor Absorption Photometers (467, 528, 652 nm) characterizing the absorption coefficient in different size ranges, an Aerodyne Cavity Attenuated Phase Shift Monitor (660 nm) and an instrument for the determination of aerosol refractive index and particle size, called OPAL.



Fig. 1: The CAPS instrument of the AEP group mounted under the wing of the NASA research aircraft DC-8 during the ATom-2 mission in February 2017.

OPAL is a highly modified airborne version of the DWOPS prototype developed by ao. Univ.-Prof. i. R. Dr. Wladyslaw Szymanski at the University of Vienna in collaboration with Dr. Aladar Czitrovsky and Dr. Attila Nagy from the Wigner Research Centre for Physics, Budapest. Besides aerosol instruments, A-HEAD is equipped with environmental sensors (temperature, pressure, relative humidity, flow) to monitor the measurement conditions, and a data acquisition system.

(3) Substantial progress was made regarding the chemical analysis of accumulation mode particles by the LAAPTOF mass spectrometer and results were presented in two recent publications: the chemical composition of radiolytic particles was reported for the first time in a paper by Dr. Anna Wonaschütz et al. (*J. Aerosol Sci.*, 2017), and the analysis of emissions from two types of mastic asphalt mixture is prepared for submission to the *Journal of Environmental Science and Technology* in a study by Weiss et al.

(4) The Vienna-type high resolution DMA (UDMA) was further developed and the resolution in the 1–2 nm size range was improved by a factor of 2.

(5) In a collaboration between the AEP group, the German Aerospace Center (DLR) and the University of Munich (LMU), a new approach to model the response of optical particle counters (OPCs) including a simple parametrization for artificial broadening of size spectra induced by the non-ideal behavior of real OPCs was developed and presented in a paper by Dr. Adrian Walser et al. (*Atmos. Meas. Tech.*, 2017). This self-consistent way allows the evaluation of calibration measurements and outlines how particle number size distributions with realistic uncertainty estimates can be derived from measured signals.

Aerosol rooftop laboratory

The aerosol measurement infrastructure in the rooftop laboratory at Boltzmanngasse 5, Vienna, was recently improved with the addition of new aerosol inlets, as well as a new data management system, allowing for automatic data storage and better accessibility. In addition, a CIMEL sun photometer – provided by the University of Valladolid (Spain, Dr. Carlos Toledano) – was installed in summer 2016 and performs measurements following the AERONET protocol. AERONET (<https://aeronet.gsfc.nasa.gov/>) is a

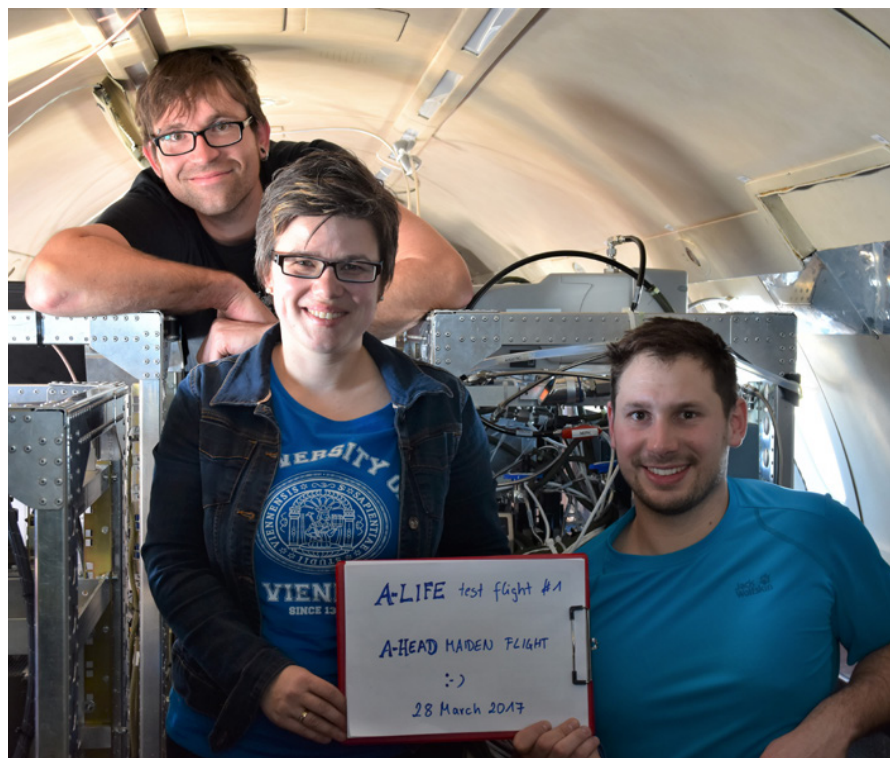


Fig. 2: Dr. Benjamin Witschas (DLR), Univ.-Prof. Dr. Bernadett Weinzierl, and Maximilian Dollner (from left to the right) in front of the new A-HEAD measurement system (right) during the A-HEAD maiden flight on 28 March 2017.

worldwide network of Cimel sun photometers providing data on the aerosol properties of the total atmospheric column. The station “Vienna_UNIVIE” belongs to the first three AERONET stations in Austria and closes a measurement gap in Central and Eastern Europe. Data from the AERONET station “Vienna_UNIVIE” are available online in near real-time.

The long-term measurements of atmospheric aerosol number size distributions and cloud condensation nuclei (CCN) using the CCN counter developed at AEP were continued and analyzed for the effect of new particle formation (NPF) events on atmospheric CCN concentrations under urban aerosol conditions in a study by Carmen Dameto et al. (*Atmos. Environ.*, 2017). Contrary to predictions from modelling studies, only a rather small effect on CCN concentrations was found. NPF events in the urban atmosphere and their possible simultaneous occurrence at different locations were also investigated (Németh et al., 2018, *Atmos. Environ.*) in a collaboration between groups from the Eötvös University Budapest (Prof. Dr. Imre Salma), and the Institute of Chemical Process Fundamentals at the Czech Academy of Sciences (Dr. Vladimír Zdimal).

Bernadett Weinzierl has been invited to join the NASA-sponsored *Atmospheric Tomography Mission* (ATom; <https://espo.nasa.gov/atom>) to study the global abundance of coarse mode aerosol and the distribution of clouds. ATom is an unprecedented field program which aims to explore the distribution of aerosols and trace gases in the background troposphere with repeated, representative profiling with the NASA DC-8 research aircraft. For ATom, the DC-8 has been equipped with multiple instrument packages collecting data of more than 350 chemical, radiative, meteorological, and microphysical parameters. ATom is a five-year program in which the NASA DC-8 research aircraft travels from near the North Pole down south the middle of the Pacific Ocean, to the Southern Ocean and Antarctica and back north over the Atlantic Ocean basin while continuously performing vertical profiles between 0.2 to 13 km altitude in four seasons. To date, three ATom deployments (summer 2016, winter 2017, autumn 2017) have been successfully completed and a unique global dataset is available. Among others, the dataset gives insight into the transport and lifetime of large mineral dust and sea salt particles under atmospheric background conditions. The last ATom deployment is scheduled for spring 2018.

ATom is led by Prof. Dr. S. Wofsy (Harvard University, Principal Investigator (PI)) and Prof. Dr. M. Prather (University of California, Deputy PI). The Science Team, comprised of 15 instrument teams and several theory teams, is led by Dr. T. Ryerson (NOAA) aided by Drs. P. Newman (NASA Goddard Space Flight Center (GSFC)), T. Hanisco (NASA GSFC), and D. Fahey (NOAA). The team from the AEP group consisting of Bernadett Weinzierl, Maximilian Dollner, Nikolaus Fölker, Harald Schuh and Mario Zak is the only non-U. S. partner in the ATom Science Team.

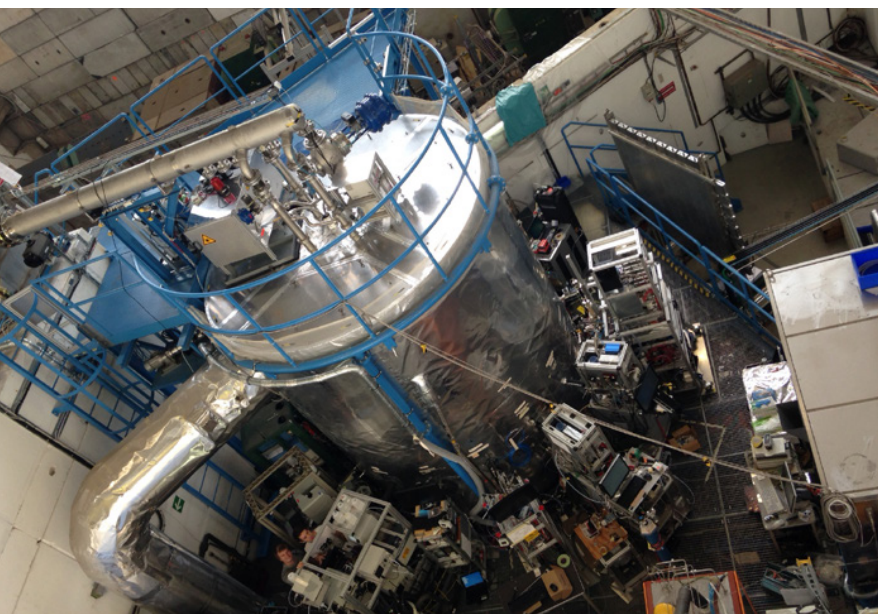


Fig. 3: Dominik Stolzenburg and Bernhard Baumgartner behind the DMA-train (left) at CERN during the CLOUD experiment at CERN.

The ERC-funded nanoDynamite team led by Ass.-Prof. Dr. Paul Winkler has meanwhile fully consolidated and is increasingly gaining visibility (see also: <http://nanodynamite.at/>). Among the main research tasks, the team continued its successful collaboration with the *Cosmics Leaving Outdoor Droplets* (CLOUD) consortium at CERN, Geneva. The newly designed DMA-train emerging from the ERC grant was tested for the first time in spring 2015 during a technical preparation run at the CLOUD chamber and was subsequently deployed at the CLOUD10 to CLOUD12 measurement campaigns in the years 2015-2017 (Fig. 3). The DMA-train has proven its potential in time-resolved nanoparticle monitoring and is meanwhile among the most important particle sizing instruments for neutral and charged particles at the well-established CLOUD project. Importantly, it bridges the gap between particle size magnifier and nano-SMPS and allows quantitative determination of growth rates in the 1.7 to 10 nm diameter range. A paper on the performance of the DMA-train has been recently published by Dominik Stolzenburg et al. (*Atmos. Meas. Tech.*, 2017). Lately, the DMA-train has also been applied to ambient measurement conditions and was involved in the A-LIFE ERC project of Bernadett Weinzierl.

The other core research task of nanoDynamite is the in-situ nanoparticle characterization by light scattering using short wavelengths. To this end, a flow tube was designed and operated during multiple beam times at the SAXS beamline of the Elettra synchrotron in Trieste, Italy. The goal is to characterize the size and shape of nanoparticles at measurement conditions close to ambient conditions utilizing x-ray scattering. Due to the low signal-to-noise ratio, primarily tungsten oxide particles were investigated exhibiting much higher electron density compared to organic particles and a differential background subtraction method was developed for low contrast sample analysis. A major breakthrough was achieved during the last beam time in September 2016 where clear scattering signals were obtained by using helium as carrier gas. Thereby the signal-to-noise ratio could be increased substantially compared to regular air. It is now possible to obtain in-situ information on particle number concentration and size at close-to-ambient particle concentrations and pressures. The SAXS experiments on the in-situ nanoparticle characterization raised quite some attention in the community and were highlighted in the first newsletter of the Central European Research Infrastructure Consortium CERIC-ERIC.

On the fundamental side of nanoparticle formation research, lab studies on the heterogeneous nucleation of n-butanol at different temperatures were performed and a new method to de-



Fig. 4: Part of the A-LIFE Science Team in front of the DLR research aircraft Falcon at Paphos airport on 27 April 2017.

termine contact angles on a scale of 1 nm from heterogeneous nucleation experiments was presented by Winkler et al. (*Sci. Rep.*, 2016). During spring 2016 the group hosted the return phase of Dr. Anne Maißer in the framework of her Erwin Schrödinger postdoctoral fellowship. One of the highlights from this period was the study of heterogeneous nucleation on sub-nanometer seed ions. It was the first time that particle formation initiated by atomic ions could be detected in the *Size Analyzing Nuclei Counter* (SANC).

The ERC project A-LIFE (2015-2020)

The ERC-funded A-LIFE project (*Absorbing aerosol layers in a changing climate: aging, lifetime and dynamics*; www.a-life.at) led by Bernadett Weinzierl has been implemented at the University of Vienna after being transferred from LMU to Vienna in March 2016. The overall aim of A-LIFE is to investigate the properties of absorbing aerosols (in particular mixtures of mineral dust and black carbon) during their atmospheric lifetime to gather a new data set on key parameters of absorbing aerosols and their distribution throughout the tropospheric column and to study potential links between the presence of absorbing particles, aerosol layer lifetime and particle removal.

A core activity within the A-LIFE project was the organization and implementation of the A-LIFE field experiment in the Eastern Mediterranean which has been successfully realized in April 2017 (Fig. 4). For A-LIFE, the DLR research aircraft Falcon has been equipped with an extensive in-situ aerosol payload including the novel A-HEAD system and the new CAPS probe, a wind lidar and meteorological sensors. The airborne measurements were complemented by ground-based in-situ and remote sensing observations in the region. Between 3 and 29 April 2017, the Falcon was based in Cyprus and carried out measurements of the entire atmospheric column from the ground up to 12-13 km in the Mediterranean. Altogether, 22 research flights (~80 flight hours) were conducted and several outbreaks of Saharan, Arabian and Middle East dust, as well as pollution, biomass burning, and dust-impacted clouds were studied. During a number of flights, coordinated observations including overflights of the ground-based sites in Cyprus (Limassol, Paphos, Agia Marina), Crete (Finokalia), and over Austria (Vienna, Sonnblick Observatory) were performed. The A-LIFE campaign was carried out in close coordination with the 18-month field observations conducted in the framework of the *Cyprus Clouds, Aerosol, and Rain Experiment* (CyCARE; October 2016 – March 2018) organized by the Leibniz Institute for Tropospheric Research (TROPOS) in Leipzig, and with the PreTECT initiative of the University of Athens.

Highlights during the A-LIFE field experiment include a sequence of six flights between 19 and 22 April 2017 which studied a Saharan dust outbreak and dust-impacted clouds between Malta, Crete and Cyprus while the dust outbreak moved eastwards across the Mediterranean. The event was also captured by the ground-based in-situ instrumentation and the lidars. Another highlight is a sequence of four flights between 26 and 29 April 2017 which investigated Arabian/Middle East dust at altitudes below 4 km and Saharan dust aloft. In most cases, a strong vertical layering of different aerosol types was observed. An unexpected observation during the measurements in the Eastern Mediterranean region was that the dust very frequently extended up to altitudes above 9-11 km.

For A-LIFE, 80 flight hours were available instead of the originally planned 40 flight hours. This was possible because two EUFAR projects were successfully acquired and clustered with A-LIFE, which provided funding for 16 additional flight hours. Furthermore, DLR provided funding for a significant amount of extra flight hours and aircraft allocation days for A-LIFE.

The analysis of the comprehensive A-LIFE data set has started. Post-campaign calibrations are ongoing and final data are under preparation. At the beginning of March 2018, the first A-LIFE data workshop will be hosted at the University of Vienna. A-LIFE involved more than 20 international partner organizations across Europe and from the U. S. From the AEP group, Sophia Brilke, Fernando Chouza, Maximilian Dollner, Nikolaus Fölker, Josef Gasteiger, Katharina Heimerl, Anne Philipp, Andrea Pölz, Harald Schuh, Christian Tauber, Marilena Teri, Clemens Weselka, Mario Zak and Bernadett Weinzierl were involved in the A-LIFE campaign by providing technical support, performing the measurements, preparing the weather forecasts, and planning the flights, respectively.

The SALTRACE project

Substantial progress was achieved with the analysis of the unique mineral dust data set from the *Saharan Aerosol Long-Range Transport and Aerosol-Cloud-Interaction Experiment* (SALTRACE; www.pa.op.dlr.de/saltrace). The airborne SALTRACE measurements in 2013 were coordinated by Bernadett Weinzierl. Specific objectives of SALTRACE were to (1) characterize the chemical, microphysical, and optical properties of mineral dust in the Caribbean, (2) quantify the impact of physical and chemical changes (“aging”) of the dust on the radiation budget and cloud microphysical processes, (3) investigate the meteorological context of transatlantic dust transport, and (4) assess the roles of removal processes during transport. The SALTRACE overview paper by Weinzierl et al. was published in the *Bull. Am.*

Met. Soc. (2017) and featured on the title page of the July 2017 Issue of BAMS. Dr. Josef Gasteiger et al. (*Atmos. Chem. Phys.*, 2017) studied particle settling and vertical mixing within the Saharan Air Layer (SAL) based on measured and modeled vertical aerosol profiles. They found evidence that vertical mixing within the SAL is a common phenomenon with significant consequences for the evolution of the size distribution and the lifetime of super-micron dust particles. Further SALTRACE results are presented in the joint SALTRACE Special Issue in the *Journal of Atmospheric Measurement Techniques/Atmospheric Chemistry and Physics* which is open for submission until 30 September 2018. To date, the SALTRACE Special Issue contains 20 publications. Further SALTRACE publications are under preparation and will be submitted within the next months.

The FWF Ice Nucleation project (2014-2018)

Within the FWF Project P26040, the ice nucleation activity of carbonaceous particles was investigated by Univ.-Prof. Dr. Regina Hitznerberger in collaboration with Prof. Dr. Hinrich Grothe, TU Vienna. Theresa Haller from the AEP group was involved in the sample preparation and analysis. In 2017, the transfer of carbonaceous particles with defined fractions of elemental and organic carbon into liquid samples was further investigated in order to gain insights into the previously unknown degree of wettability of freshly produced combustion soot. The internal structure of these particles was investigated using Raman scattering and transmission electron microscopy to track the changes of the degree of graphitization of the particles during thermal treatment analogous to typical thermo-optical analysis of elemental and organic carbon in ambient aerosols. Within the collaboration in the FWF project, further investigation of the ice nucleating abilities of these laboratory-generated soots and various biological particles was performed.

The Marie Curie International Training Network (ITN) VERTIGO (2014-2017)

Work on the VERTIGO project (<http://www.vertigo-itn.eu/>) was continued. VERTIGO is an interdisciplinary research network coordinated by Dr. Ulrich Küppers (LMU) which aims to study the physico-chemical processes during the lifecycle of volcanic ash. Bernadett Weinzierl coordinates the VERTIGO sub-project dealing with an improved detection of volcanic ash mass concentration from airborne observations. Important progress was made in the understanding of flow distortion effects introduced by the fuselage of an aircraft on aerosol instruments mounted under the aircraft wing. A correction scheme for size-dependent particle concentration errors and droplet-deformation of open-stream aerosol and cloud probes on fast-flying aircraft has been

developed and a manuscript is currently being prepared by Antonio Spanu et al. for submission to the *Journal of Atmospheric Measurement Technology*.

Field observations with a polar nephelometer and a telephotometer

In June 2016, Univ.-Prof. i. R. Dr. Helmuth Horvath conducted measurements with a polar nephelometer in the Sierra Nevada to determine the volume scattering function of Saharan aerosol. In a second field experiment in July and August 2017, Helmuth Horvath and Paulus Bauer performed measurements of the extinction coefficient in the Boulder/Denver area (Colorado, USA). The overall aim of the field experiment in Boulder was to repeat observations from the year 1979 to investigate potential changes in the aerosol composition and load between 1979 and 2017. Both, the measurements in 1979 and 2017, were performed with the identical telephotometer designed at the University of Vienna.

Nano-particle observations with DMA systems

Significant advancement was made with the generation of electrically neutral molecular clusters. In a study by Dr. Gerhard Steiner et al. (*Aerosol Sci. Technol.*, 2017) which is based on measurements performed in the framework of a workshop at the University of Helsinki in 2015, two novel techniques for the generation of well-defined ionic molecular clusters as test aerosols for calibration purposes and for basic studies at the molecular level were presented. The results will allow a step forward in the quantitative measurement of atmospheric charged and neutral clusters with the CI-API-TOF-MS.

With the nanoTOF, a mass spectrometer specially designed to gather mobility-resolved information about the chemical composition of atmospheric cluster ions became recently available. First ambient-air measurements with the Innsbruck nanoTOF, were carried out during the nanoTOF-IBK measurement campaign in 2016/2017, initiated by Gerhard Steiner, as well as during subsequent measurements in down-town Innsbruck in collaboration with Prof. Dr. Thomas Karl. The AEP group supported the measurements with a DMPS system and a water-based laminar flow CPC which allowed the determination of the particle size distribution in the size range between 10 nm and 1000 nm, as well as the total number concentration of particles.

The Vienna-type high resolution UDMA is also key instrument in a collaboration with Ionicon Analytik GmbH initiated by Gerhard Steiner. In the framework of this collaboration, state-of-the-art mass spectrometers were calibrated,

and measurements at the CLOUD12 campaign at CERN were performed with the UDMA and the Ionicon IoniAPI-TOF.

New projects

Besides the projects described earlier in this report, an EU-funded Marie Curie ITN (CLOUD-MOTION) in which Paul Winkler is partner, and two COST Actions in which Bernadett Weinzierl is partner were recently approved (CA 2016-1-20692/COLOSSAL: *Chemical On-Line cOmpoSition and Source Apportionment of fine aerosol*; 2017-CA16202, InDust: *International Network to Encourage the Use of Monitoring and Forecasting Dust Products*). Furthermore, three Erwin Schrödinger fellowships were granted to Agnieszka Kupc (now at: U. S. Department of Commerce, National Oceanic and Atmospheric Administration (NOAA), Boulder, USA), Bernadette Rosati (now at: University of Aarhus, Aarhus, Denmark), and Daniela Wimmer (now at: University of Helsinki, Finland).

Dissemination and Collaborations

The group's scientific activities and accomplishments are documented in numerous peer-reviewed publications and presentations at international conferences, and have been internationally acknowledged by the fact that various group members presented a large number of invited or platform presentations and posters at international conferences, universities and research institutes in Europe, the United States and Asia or acted as key note speakers (e. g. at the Symposium of the *Nordic Society for Aerosol Research* in 2016). Results and scientific activities are also shared in different blogs (<http://aerosols.univie.ac.at/blogs/>; <http://nanodynamite.at/blog.html>).

Since 2015, 78 peer-reviewed articles were published including high-impact papers in *Nature* (3), *Nature Scientific Reports* (1), *Science* (1), *PNAS* (1), *Geophys. Res. Lett.* (1), and *Bull. Am. Met. Soc.* (3). We have thereby gained substantial media presence: Paul Winkler was on broadcast in Austrian TV about aerosol nucleation without sulfuric acid. Profs. Dr. Paul Wagner and Paul Winkler contributed to a TV science magazine ("Newton") which discussed the physics of clouds in the context of climate change. The long-term measurements of aerosol size distributions at the rooftop laboratory were presented in the Ö1 "Mittagsjournal" by Anna Wonaschütz. Bernadett Weinzierl gave interviews for BBC and the Ö1 "Morgenjournal" discussing how biofuel blending may reduce particle emissions from aircraft engines at cruise conditions. She was also a guest in the live radio show "Punkt Eins" (Ö1) where listeners discussed observations and properties of clouds with her. She contributed

to the radio show “Rudi Radiohund” (Ö1) which raised the question “Why does the sky appear in different colors?”. Together with colleagues from NASA and the Harvard University, Bernadett Weinzierl talked in a NASA photo postcard on YouTube about the mineral dust measurements during ATom.

Besides contributions on TV and on the radio, several newspaper articles, including articles in “Die Presse” or the magazine of the “Junge Akademie” at the Berlin-Brandenburg *Academy of Sciences and Humanities and the German National Academy of Sciences Leopoldina*, featured results achieved within the framework of the ATom mission, the CERN CLOUD collaboration and the NASA-DLR biofuel measurements. Results of the research in the AEP group were also presented to the broader public, for example with presentations at the Deutsches Museum Munich in the framework of the series “Wissenschaft für Jedermann”, the Körber Forum, a panel discussion at the Natural History Museum Vienna, and the Junior Science Club.

The work of the AEP group has also been acknowledged with two scientific awards: Bernadett Weinzierl received the NASA Group Achievement Award 2016 for outstanding achievement conducting multi-aircraft experiments demonstrating benefits of renewable jet fuel in reducing air quality and climate impacts of aviation. Dr. Fernando Chouza was awarded with the third prize in the category dissertations of the Green Photonics Young Talent Award 2017 for his dissertation (supervisors: Dr. Oliver Reitebuch (DLR) and Bernadett Weinzierl).

As can be seen from our publications, much of the work is originating from highly productive international collaborations. The most active collaborations in the past few years have been with the CLOUD, ATom, SALTRACE and A-LIFE consortia, including extensive collaborations with various U.S. and European research groups at Harvard University, National Oceanic and Atmospheric Administration (NOAA), NASA, University of Minnesota, University of California, Irvine, Brookhaven National Laboratory, DLR, LMU, TROPOS, and the University of Helsinki.

Further activities included services of group members in various review panels e. g. from the *Finnish Academy of Sciences*, committees such as the membership in the board of the *Association for Aerosol Research* (GAeF) where Helmuth Horvath is president and Bernadett Weinzierl vice-president for the period 2016-2018, as well as editorial board memberships of Wladyslaw Szymanski at “Particuology”, and “Aerosol and Air Quality Research”, and Regina Hitzemberger at “Journal of Aerosol Science” and “Air Quality, Atmosphere & Health”.

In order to share the most current aerosol science research achievements and expertise, the AEP group regularly holds international Summer Schools on aerosol science. The fifth and sixth univie:summer school “*Basic Aerosol Science*” took place from 4 to 11 July 2015 (organizer: Helmuth Horvath) and from 10 to 15 July 2017 (organizer: Bernadett Weinzierl), respectively. The summer school was established in 2007 and offers a broad education in basic principles and techniques in the field of aerosol science needed to understand and critically review aerosol processes and their interaction with the environment. Besides lectures, the participants have time for discussions, and participate in a 1-day field experiment measuring the atmospheric extinction coefficient on the Hohe Wand mountain near Vienna. The summer school targets international graduate students and early post-doctoral researchers, as well as persons who work in the field of aerosol science. In 2015 and 2017, 20 and 19 participants from 9 different countries attended the univie:summer school “*Basic Aerosol Science*”, respectively.

The international reputation of the AEP group is underlined by frequent visits of highly recognized scientists from Europe, North America and Japan. Among others it was a great pleasure to welcome the following colleagues: Dr. Charles A. Brock (NOAA, Boulder, USA), a close collaborator of the AEP group in the framework of the ATom mission gave a talk in our seminar; Prof. Dr. Peter McMurry (University of Minnesota, USA) gave a lecture in our seminar and acted as a referee at the defense of T. Pinterich’s PhD thesis; Prof. Dr. Ina Tegen (TROPOS, Germany), the head of the TROPOS modelling department and a close collaborator in the framework of mineral dust research, gave a presentation in our seminar and joined together with Bernadett Weinzierl the panel discussion “Umwelt im Gespräch: Wie Feinstaub das Klima beeinflusst” at the Natural History Museum in Vienna. We also welcomed Prof. Dr. Masami Furuuchi and Prof. Dr. Tohno (Kanazawa University, Japan) for an exchange visit in the framework of an official Memorandum of Understanding between Kanazawa University and the Faculty of Physics coordinated by AEP. In April 2016, a preparatory workshop for the implementation of the A-LIFE field experiment with about 20 visitors from different European institutions was hosted by the AEP group. Furthermore, a collaborative visit of about 35 international guests took place during a CLOUD workshop held at the University of Vienna in May 2017. At this occasion Prof. Dr. Joachim Curtius from the Goethe University Frankfurt gave a talk at the Chemical-Physical Society. In addition, CLOUD spokesperson Dr. Jasper Kirkby was invited as speaker at the Vienna Physics Colloquium in December 2016 by the Vienna Doctoral School in Physics. The visit was organized and hosted by PhD students from the AEP group.

The AEP group not only hosted visitors, but the group members were also invited to other institutes. For example, Wladyslaw Szymanski was invited as a senior visiting professor at the Kasetsart University, Bangkok (Thailand) for the January – April periods in 2015, 2016, 2017, and 2018.

Selected publications

Dameto de España, C., A. Wonaschütz, G. Steiner, B. Rosati, A. Demattio, H. Schuh, and R. Hitznerberger, 2017: Long-term quantitative field study of New Particle Formation (NPF) events as a source of Cloud Condensation Nuclei (CCN) in the urban background of Vienna. *Atmosph. Env.*, 164, 289-298, doi:10.1016/j.atmosenv.2017.06.001.

Gasteiger, J., S. Gross, D. Sauer, M. Haarig, A. Ansmann, and B. Weinzierl, 2017: Particle settling and vertical mixing in the Saharan Air Layer as seen from an integrated model, lidar, and in situ perspective. *Atmos. Chem. Phys.*, 17, 297-311, doi:10.5194/acp-17-297-2017.

Kirkby, J., J. Duplissy, K. Sengupta, C. Frege, H. Gordon, C. Williamson, M. Heinritzi, M. Simon, C. Yan, J. Almeida, J. Tröstl, T. Nieminen, I. K. Ortega, R. Wagner, A. Adamov, A. Amorim, A.-K. Bernhammer, F. Bianchi, M. Breitenlechner, S. Brilke, and Coauthors, 2016: Ion-induced nucleation of pure biogenic particles. *Nature*, 533, 521-526, doi:10.1038/nature17953.

Moore, R. H., K. L. Thornhill, B. Weinzierl, D. Sauer, E. D'Ascoli, J. Kim, M. Lichtenstern, M. Scheibe, B. Beaton, A. J. Beyersdorf, J. Barrick, D. Bulzan, C. A. Corr, E. Crosbie, T. Jurkat, R. Martin, D. Riddick, M. Shook, G. Slover, C. Voigt, and Coauthors, 2017: Biofuel blending reduces particle emissions from aircraft engines at cruise conditions. *Nature*, 543, 411-415, doi:10.1038/nature21420.

Steiner, G., A. Franchin, J. Kangasluoma, V. M. Kerminen, M. Kulmala, and T. Petäjä, 2017: Production of neutral molecular clusters by controlled neutralization of mobility standards. *Aerosol Sci. Technol.*, 51, 946-955, doi:10.1080/02786826.2017.1328103.

Stolzenburg, D., G. Steiner, and P. M. Winkler, 2017: A DMA-train for precision measurement of sub-10 nm aerosol dynamics. *Atmos. Meas. Tech.*, 10, 1639-1651, doi:10.5194/amt-10-1639-2017.

Tröstl, J., W. K. Chuang, H. Gordon, M. Heinritzi, C. Yan, U. Molteni, L. Ahlm, C. Frege, F. Bianchi, R. Wagner, M. Simon, K. Lehtipalo, C. Williamson, J. S. Craven, J. Duplissy, A. Adamov, J. Almeida, A.-K. Bernhammer, M. Breitenlechner, S. Brilke, and Coauthors, 2016: The role of low-volatility organic compounds in initial particle growth in the atmosphere. *Nature*, 533, 527-531, doi:10.1038/nature18271.

Weinzierl, B., A. Ansmann, J. M. Prospero, D. Althausen, N. Benker, F. Chouza, M. Dollner, D. Farrell, W. K. Fomba, V. Freudenthaler, J. Gasteiger, S. Groß, M. Haarig, B. Heinold, K. Kandler, T. B. Kristensen, O. L. Mayol-Bracero, T. Müller, O. Reitebuch, D. Sauer, and Coauthors, 2017: The Saharan Aerosol Long-Range Transport and Aerosol-Cloud-Interaction Experiment: Overview and Selected Highlights. *Bull. Am. Met. Soc.*, 98, 1427-1451, doi:10.1175/bams-d-15-00142.1.

Winkler, P. M., R. L. McGraw, P. S. Bauer, C. Rentenberg, and P. E. Wagner, 2016: Direct determination of three-phase contact line properties on nearly molecular scale. *Sci. Rep.*, 6, 26111, doi:10.1038/srep26111.

Wonaschuetz, A., P. Kallinger, W. Szymanski, and R. Hitznerberger, 2017: Chemical composition of radiolytically formed particles using single-particle mass spectrometry. *J. Aerosol Sci.*, 113, 242-249, doi:10.1016/j.jaerosci.2017.07.012.

Basic Experimental Physics Training and University Didactics

General

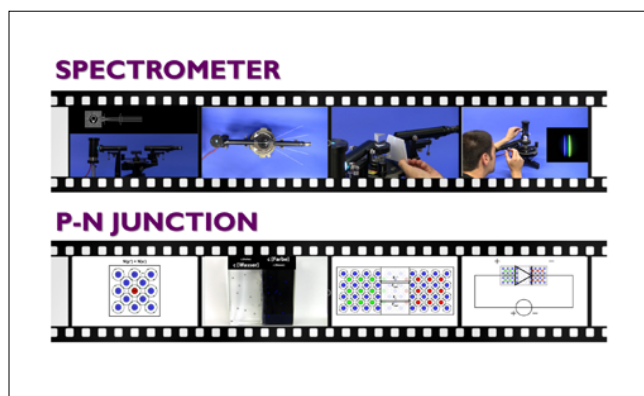
Our main tasks are basic experimental physics training, experimental courses and scientific aspects of teaching and learning, cooperating closely with the group Workshop and Technical Services and the Austrian Educational Competence Centre Physics (AECCP).

Most academic members are also affiliated with other research groups. For details, see our website <http://teaching-physics.univie.ac.at>.

In January 2015 Ewa Partyka-Jankowska joined the group as a technician for the introductory lectures. Heinz Kabelka's vacant position was filled by two half-time senior lecturers: In October 2015 Jürgen Klepp started supervising groups of "Exercise course in Introductory Physics I" and in February 2016 Lana Ivanjek started running the physics teaching lab. Heinz Kabelka had taught students how to conduct experiments in the classroom in the "High school teaching lab" for many years. He kindly continued teaching in this lab for two more winter semesters and assisted in providing a number of experiments for the lectures "Introduction to Physics I and II".

In February 2017 Daria Setman became half-time senior lecturer in the introductory physics lab, as Alfred Korner, who was very engaged in the introductory physics lab, retired in October 2017. At the same date Romano Rupp retired but he is still giving the lectures "Introduction to Physics I and II".

The teacher training programme is currently undergoing major changes with respect to the curriculum and its organization, which is a substantial challenge for all of us.



Videos on spectrometers and pn-junctions.

Introductory Physics Lab and Teaching

In the introductory physics lab, several new experiments were developed, evaluated and successfully implemented. For example, an old but strong electromagnet facility was adapted to measure the susceptibility parameters of para- and diamagnetic samples, and an interesting and easy-to-handle experiment about the Hall effect as well as a new monoenergetic gamma-ray-absorption experiment by using a CS-137 source were developed. Furthermore, a new lab course setup was developed and tested in summer term 2015. Positive evaluation encouraged a second/new adapted lab course for teacher candidates in winter term 2015. Moreover, Clemens Nagel held the lecture "physics for chemistry teacher candidates" for the first time and tested a peer-instruction¹ setup with clicker questions in between the teacher-oriented phases. This setup aims at a better understanding of the basic concepts in several fields of physics.

In 2015, four videos were produced, implemented and scientifically evaluated. Two of them will help students handle complex experimental setups: prism and grating spectrometers as well as digital storage oscilloscopes.

The other two explain difficult basic concepts: p-n junctions and electric circuit physics.

During 2016 and 2017, the curriculum for BSC Physics was restructured by the CurrAG. In parallel, Clemens Nagel and Wilhelm Markowitsch developed a new 3-fold structure for the basic experimental lab courses taking into account that a higher number of students have to achieve knowledge and abilities at at least the same scientific and pedagogical quality level.

The eLearning part of the lab course for nutritional scientists was transferred to the Moodle platform during 2017.

¹ Mazur, E. Peer Instruction: a user's manual. (Prentice Hall, 1997)

Open House Day

One highlight of the year 2015 were the hands-on activities at the Faculty's Open House Day in June. Over 100 people performed various experiments from everyday life, e. g. the gummy bear wave machine. Ewa Partyka and Franz Sachslehner guided 120 pupils in 8 groups through the historical collection and provided a guided tour to about 60 additional people in the evening.



Open house day: Ewa Partyka presents the historical collection (left). Gummy bear wave machine (top right), imitation of velocity-time curves in the introductory lab (bottom left).

Project “SOLARbrunn”

The two-year Sparkling Science project “SOLARbrunn – Heading for a future powered by the sun” of Ilse Bartosch focuses on the development of a regional energy concept for Hollabrunn (a town with 12,000 inhabitants) using the public kindergarten building as a model. Students of the Higher College of Engineering (HTL) in Hollabrunn did research in the context of their A-level thesis supported by their teachers, an interdisciplinary research team consisting of Ilse Bartosch (physics didactics), Viktor Schlosser (physicist) and Anna Streissler (social scientist, Forum Umweltbildung), and teacher candidates. Key to finding the right answers for enhancing the comfort at the kindergarten was a continuous discourse with the municipal stakeholders, which gave rise to critical thinking about “passionate engineering”, but also to discussions of further organisational development opportunities for making STEM education (Science, Technology, Engineering and Mathematics) in general and HTLs specifically a more welcoming field for girls.

On 22 November 2016 this project was honoured with the “Education for sustainable development – BEST OF AUSTRIA” award. On 13 June 2016 the “Ars Docendi-Staatspreis for excellent teaching 2016” was awarded to Franz Embacher in the category “Digital teaching and learning elements in connection with traditional forms of teaching”. This award concerned the lectures on the mathematical basics for the studies of physics.

Lecture Halls

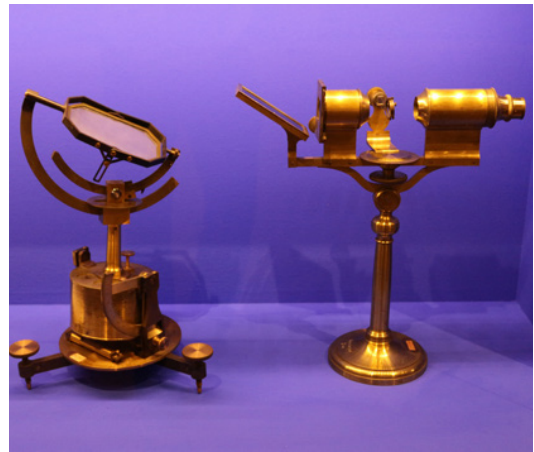
In 2015, the Ernst Mach Lecture Hall, the Erwin Schrödinger Lecture Hall and the Seminar Room on the 5th floor were renovated and equipped with new variable tables and chairs. The Ernst Mach Lecture Hall, in particular, can be adapted to the special needs of larger meetings, conferences and poster presentations. Because of the high numbers of beginning students the Lise Meitner Lecture Hall was equipped with modern streaming technology during summer 2016. This was also a pilot project for the IT services unit of the University of Vienna, as a new and better streaming technology was applied.

Historical Collection

On 17 January 2015 the Faculty of Physics arranged the matinee “The success of the Viennese Physics – from the Physical Museum to the Nobel Prize” in four sessions. The lectures were given by Walter Kutschera, and Franz Sachslehner guided ~100 visitors through the Faculty’s historical collection.



Matinee: Presentation of the historical collection by Franz Sachslehner.



Historical objects at the exhibition “Das Wissen der Dinge”.

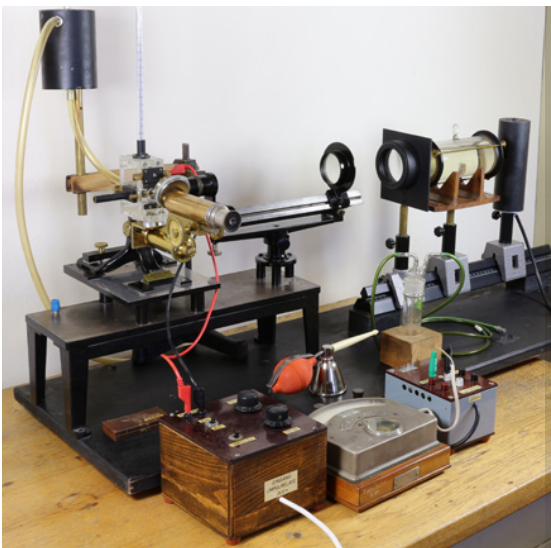
In 2015, two Tesla transformers from around 1900 were lent to the artist Eva Mayr for the exhibition “Tesla revisited” during the Biennale in Venice. Furthermore the “ice calorimeter after Lavoisier” and an old dewar for liquid air have been exhibited in the Museum der Heizkultur Vienna since September 2017 (“Friert euch nicht – eine Reise unter Null”).

For the 650th anniversary of the University of Vienna, Claudia Feigl designed the exhibition “Das Wissen der Dinge” at the Museum of Natural History, Vienna, using historical objects from different scientific disciplines, including some 19th-century objects from the Faculty’s historical collection.

2016, a considerable number of devices from the “Physical Collection of the HTL Wien Ottakring” were transferred officially to our faculty’s physical collection as a permanent loan. Some of these objects are presented in a separate showcase. In this year the Ehrenhaft-Millikan experiment of the former advanced lab course was also handed to the historical collection. The optical parts of this experiment are still from Felix Ehrenhaft’s era. Some missing parts of the elementary electrical charge measurement are at the Vienna Technical Museum. There, kindly supported by A. Veiter and I. Brucha, Franz Sachslehner was permitted to photograph all available objects of Ehrenhaft’s experiments, such as a three-level recorder and a replica of the original Ehrenhaft condenser of 1914.



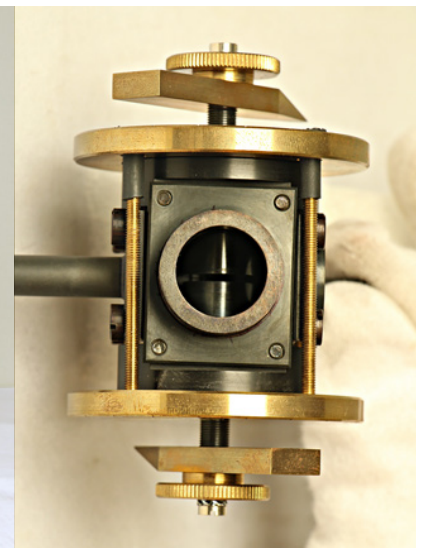
Permanent loans of the HTL Ottakring, Vienna – left to right: showcase with Atwood machine, tangent galvanometer, Geryk double-cylinder vacuum pump.



Ehrenhaft-Millikan experiment of the former advanced lab course.



Ehrenhaft's three-lever recorder (original) and condenser (replica) from around 1914, kept by the Vienna Technical Museum.



300 Years of Experimental Physics at the University of Vienna

In 2015, Franz Sachslehner succeeded in locating the little-known “foundation paper” of the Musaeum mathematicum. Founded in 1714, it became the earliest base for extended experimental – mostly physics – equipment. In the mid-18th century its name changed to “Physikalisches Museum”. Together with the Chair of Physics it existed in the traditional form until 1850 and served as the starting point for future Viennese physics.

Subsequently, in 2016 and 2017, Franz Sachslehner gave a series of three talks on “300 years experimental physics at the University of Vienna”. The first part covered the period from 1714 – 1850 (see record at <http://phaidra.univie.ac.at/o:426678>), the second from 1850 – 1920 (<http://phaidra.univie.ac.at/o:448220>) and the third from 1920 until today (<http://phaidra.univie.ac.at/o:515896>).

Computational Materials Physics

Mission

The main research efforts of our group are directed towards the development of quantum mechanical tools for atomic scale simulations of properties and processes in materials, and the application of these methodologies to key areas of materials research. An important pillar of our research is the Vienna *Ab initio* Simulation Package (VASP), a general *ab initio* code for solving the many-electron Schrödinger equation. It is suitable for the simulation of materials properties of solids, surfaces, as well as molecules. The VASP code is among the world leaders in its field and particularly well suited for the simulation of condensed matter systems. The last years continued to be strong years with about 200 new licenses every year, with the total number of licensees now being over 3000. This is a great success but also an obligation for us to continue serving the steadily growing user community, thriving to improve the user friendliness of VASP by adding new functionalities, and making VASP fit for the next generation of computing platforms.

Our research is currently focused on developing important post-density functional theory methods that allow for a more accurate description of the correlation energy, for instance many-body perturbation theory. The code development, maintenance and support of our steadily increasing user community are handled by Doris Vogtenhuber, Martijn Marsman, Merzuk Kaltak and Ferenc Karsai. For the code development, we now witness a strong shift from CPUs (central processing units) with few cores towards CPUs with many, possibly hundreds of cores. Likewise, graphic processing units (GPUs) are becoming increasingly popular in high performance computing. This requires a substantial redesign of many features of the code, which is actively tackled by the lead developer Martijn Marsman in close collaboration with Intel and NVidia.

The techniques developed in the group are applied to a wide range of current problems in solid state physics and materials science covering the following areas:

- surface science and catalysis,
- semiconductors and insulators including solar cells,
- magnetism and magnetic nanostructures,
- quantum materials,
- strongly correlated oxides,
- minerals (including zeolites, clays, and ceramics).

What is new

Several students finished their PhD work in this reporting period, including Leif Eric Hintzsche, Merzuk Kaltak, Felix Hummel, Peitao Liu and Tobias Sander. With Benjamin Ramberger, Tobias Schäfer, Thomas Hahn, Jonathan Lahnsteiner, Zeynep Ergonenc, Michele Reticioli and Manuel Engel we have hired new outstanding PhD students. Furthermore, Menno Bokdam has been appointed as University Assistant strengthening our research in the area of novel solar cell materials.

The most important personnel developments are the appointment of Cesare Franchini to full Professor in 2017 and the appointment of Kerstin Hummer to Associated Professor in 2016. Cesare Franchini also received a "Shield of Honor" at the Abbottabad University in Pakistan. We also congratulate one former PhD, Andreas Grüneis, who has been appointed as a full professor at the Technical University of Vienna.

The core of our research continues to be anchored in the FWF-Spezialforschungsbereich **ViCoM** (Vienna Computational Materials Laboratory), headed by Georg Kresse as speaker. The research groups of Cesare Franchini and Kerstin Hummer are both flourishing. Cesare Franchini has acquired his third FWF funded project covering the intriguing physics of polarons (collaboration with Belgium), and Menno Bokdam has received a grant to perform research on novel solar cell materials. Our group is also actively participating in knowledge transfer and outreach activities of the faculty. A special concern of Kerstin Hummer are activities that counteract the gender segregation in natural sciences, informatics and technology at younger ages.

Highlights 2015-2017

Our group published about 70 papers in international peer-reviewed journals in 2015-2017. Furthermore, the members of the group presented about 120 invited lectures, seminar talks and posters.

Accurate description of correlation beyond mean field approximations

Research on the improved description of electronic correlation continued to be a strong focus. The research has, however, shifted from an evaluation of the methods towards making the methods routinely applicable to solid state problems. This is tenuous work but required to establish these methods for a wider community. For instance, we were able to improve the scaling down to cubic in system size, making the codes routinely applicable to supercells of several hundred atoms. Furthermore, we improved the methods quantitatively so that they are now capable of predicting physisorption energies with a few percent accuracy. On the methodology side, we were able to derive and implement forces in the random phase approximation, a first-time achievement in solid state physics [1]. We applied this methodology to test density functionals for important novel solar cell materials (MAPbI_3 , see Fig. 1). These materials have recently reached a light to electricity conversion efficiency of 20 % [2].

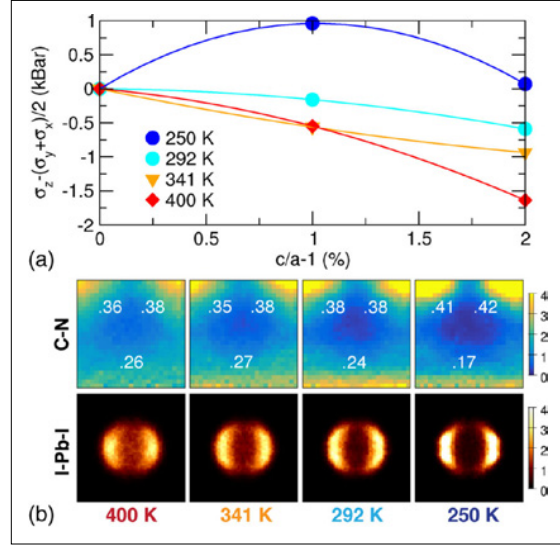


Fig.1: (a) Stress difference in the tetragonal MAPbI_3 system as a function of c/a ratio and temperature. The blue line shows that the tetragonal phase is preferred at low temperature. (b) Structural evolution showing that molecules are aligned parallel to the xy plane at low temperature.

Quantum material modelling

This line of research, led by Cesare Franchini, is directed towards the description of correlated oxides including surfaces. The studies focus on the interplay of different competing interactions, for instance spin-orbit and electron-phonon couplings. These can lead to the onset of novel quantum states, phase transitions and innovative applications. A representative work of the role of spin-orbit interaction was the study on relativistic anisotropic magnetic interactions in Sr_2RuO_4 and their effect on the superconducting order parameter, published in the Nature journal Quantum Materials [3]. The main highlight on the importance of electron-phonon interactions is the study on the polaron-mediated structural reconstruction of the $\text{TiO}_2(110)$ surface published in PRX, also highlighted in Nature Review Materials [4] (Fig. 2).

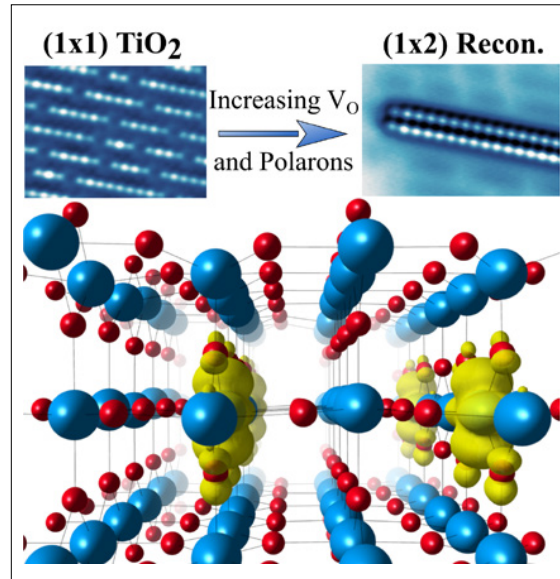


Fig. 2: Surfaces can undergo reconstructions to minimize their free energy. In this work, we have shown that this process can be mediated by polaronic quasiparticles, formed by the coupling of excess electrons and the local phonon field. We found that this process is in action in the polaron materials TiO_2 which undergoes a 1×1 to 1×2 transition with increasing number of polarons (in this case generated by oxygen vacancies).

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- [2] M. Bokdam, J. Lahnsteiner, B. Ramberger, T. Schäfer, and G. Kresse, Phys. Rev. Lett. 119, 145501 (2017). 10.1103/PhysRevLett.119.145501
- [3] B. Kim, S. Khmelevskiy, I. Mazin, D. Agterberg, C. Franchini, npj Quantum Materials 3, 37 (2017). doi:10.1038/s41535-017-0041-8
- [4] M. Reticcioli, M. Setvin, X. Hao, P. Flaue, G. Kresse, M. Schmid, U. Diebold, and C. Franchini, Phys. Rev. X 7, 031053 (2017). 10.1103/PhysRevX.7.031053

Computational Physics

The Computational Physics Group uses modern computer simulation techniques combined with analytical theory to study a broad range of condensed matter systems with an emphasis on soft matter and the statistical mechanics of equilibrium and non-equilibrium processes. Research topics include complex fluids, macromolecules, colloids, nanocrystals, phase transitions, dynamical instability of classical many-body systems, transport processes and systems far from equilibrium, as well as quantum mechanical many-body systems.

What's new

In the period of this report, several people joined the group and new international projects have started. Diego Jaramillo, Michela Ronti and Andrei Bazarenko started working towards their doctoral degrees as Early Stage Researchers in the ETN-COLLDENSE coordinated by Sofia Kantorovich. David Toneian joined the group as PhD student, jointly with the group of Prof. G. Kahl at the TU Wien, within the framework of the SFB-ViCoM. Lisa Weiß joined the group to start working towards her doctoral degree as an Early Stage Researcher in the ETN-NANOTRANS, which was approved by the EU in 2015. Max Innerbichler joined the group as PhD student funded from an FWF project. Ioana Cristina Garlea and Marcello Sega both joined the group as University Assistants. Tobias Morawietz took up a postdoc position funded by the SFB-ViCoM and Luca Tubiana started as a postdoc in the INDICAR project. Markus Hartmann came to the group on a postdoc position funded through his own FWF project, which also funds Huzaifa Shabbir, who joined the group as a doctoral student. Gyorgy Hantal came to the group as Marie-Curie Fellow. A new grant “The Art of Magnetism” was awarded to Sofia Kantorovich and her group by the FWF within their new program on science communication.

A number of visitors spent extended times in the group, including PhD students Andreas Doukas from Ljubljana, Martina Foglino from Edinburgh, José Manuel Ruiz from Rome La Sapienza as well as PostDocs Elena Pyanzina, Ekaterina Novak and Alla Dobroserdova from the Ural Federal University and the visiting Professor Alexey Ivanov. Koen Marinus from TU Eindhoven spent 4 months as an Erasmus student in the group and Phill Geissler from UC Berkeley visited the group for an extended period in the spring of 2017.

Christian Leitold and Peter Poier were awarded their PhD degrees with Highest Honors and in March 2017 they received their Doctoral Diploma *sub auspiciis praesidentis rei publicae*. Maximilian Liebetreu obtained a highly competitive uni:docs PhD Fellowship to perform work on the shear properties of knotted polymer solutions. During the 2nd Erwin Schrödinger Symposium 2016, Lorenzo Rovigatti, Lise Meitner Fellow in the group, was awarded the 2016 Nano Prize of the Erwin Schrödinger Society for Nanosciences. Michela Ronti was awarded a poster prize for her work on the phase behavior of dipolar hard spheres that she presented during the EMLG conference in September 2017.

In December 2015, Prof. Likos was awarded the *Sofronios-Elias Papadopoulos Prize* of the Department of Physics, of the School of Applied Mathematical and Physical Sciences of the National Technical University of Athens. The prize, which was awarded for the first time, honors the memory of a great colleague and teacher. The prize recognizes the impact of Likos' continuous scientific research efforts, as well as his devotion and commitment to academic excellence in the field of Condensed Matter Physics.

Christos Likos has been elected Member of the National Research and Innovation Council of Greece and in 2017 his tenure as Associate Editor of Soft Matter was renewed for additional three years.

Ivan Coluzza, Swetlana Jungblut, Sofia Kantorovich and Marcello Sega obtained their habilitation, which now permits them to officially supervise students.

Since the beginning of 2017, Christoph Dellago is the Director of the Erwin Schrödinger Institute for Mathematics and Physics at the University of Vienna, which hosts numerous scientific workshops, thematic programs and summer schools every year.

In the fall of 2016, Prof. Martin Neumann retired after many years of dedicated teaching and research at the University of Vienna.

The group organized several workshops and conferences, including the CECAM/ESI Workshops “From trajectories to reaction coordinates: making sense of molecular simulation data”, “Interactions and Transport of Charged Species in Bulk and at Interfaces”, “Water at interfaces: from proteins to devices”, “Challenges across Large-Scale Biomolecular and Polymer Simulations”, and “Physics and Chemistry at Fluid/Fluid Interfaces”, which took place at the Erwin Schrödinger Institute for Mathematics and Physics. In 2016, the group organized MECO 41, the Annual Meeting of the Middle European Cooperation in Statistical Physics as well as the Annual Meeting 2016 of the Austrian Physical Society. Group members also actively participated in the 650th Anniversary of the University of Vienna. Sofia Kantorovich's research was highlighted by hyperraum.tv in Munich.

Research Highlights

“Validity of the Stokes-Einstein relation in soft colloids up to the glass transition”

by S. Gupta, J. Stellbrink, E. Zaccarelli, C. N. Likos, M. Camargo, P. Holmqvist, J. Allgaier, L. Willner, and D. Richter, *Phys. Rev. Lett.* **115**, 128302 (2015).

Glasses feature properties that are in many ways controversial. Their microscopic structure is akin to that of a fluid but their mechanical properties are those of a solid. Close to the glass transition, the microscopic and macroscopic properties of glass-forming systems also show unusual behavior. Contrary to usual fluids, the viscosity of the system cannot any more be determined by the diffusion of individual particles. The connection between the two, known as Stokes-Einstein relation, breaks down in the vast majority of glasses, presumably due to the presence of strong dynamical heterogeneities in the system. In a broad collaboration, bringing together experimentalists in Jülich and theorists in Rome, Cali, and Vienna, a new class of soft colloids that display a glass transition has been investigated, using scattering techniques, theory and simulation. It has been found, by direct, parameter-free comparison of experimental and theoretical results, that these glasses are different: the Stokes-Einstein relation remains valid for them all the way to the glass transition. These findings bring forward an experimental realization of the scenario of ultrasoft glasses, which has been hypothesized to conform to the Stokes-Einstein relation due to suppression of dynamical heterogeneities [1]. The work has been highlighted in a *Focal Point* article in the *Physik Journal* by the German Physical Society [2].

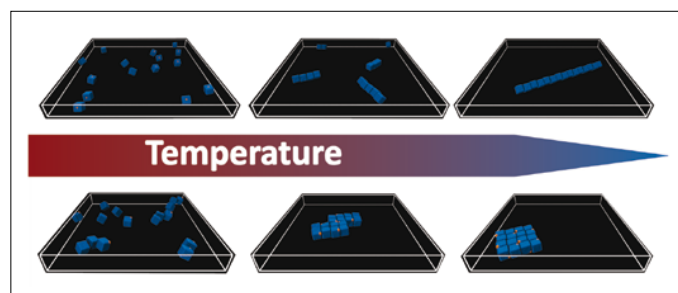
[1] A. Ikeda and K. Miyazaki, *Phys. Rev. Lett.* **106**, 015701 (2011).

[2] M. Fuchs, *Physik Journal* **14** (12), 20 (2015).

“Directional self-assembly of permanently magnetised nanocubes in quasi two dimensional layers”

by J. G. Donaldson and S. S. Kantorovich, *Nanoscale* **7**, 3217 (2015).

Here, we have investigated the systems of dipolar nanocube monolayers. Using an applied analytical approach, in combination with molecular dynamics simulations, we have determined the ground state structures of individual monolayer clusters. We discovered that the structure of the ground state is distinctly different for the two systems of permanently magnetised nanocubes; [001] cubes form dipolar chains in the ground state, whereas those with [111] orientation adopt square lattice structures. The discovered configurations in the ground state represent two different structural motifs, as yet unobserved in the ground state of other magnetic nanoparticle systems.

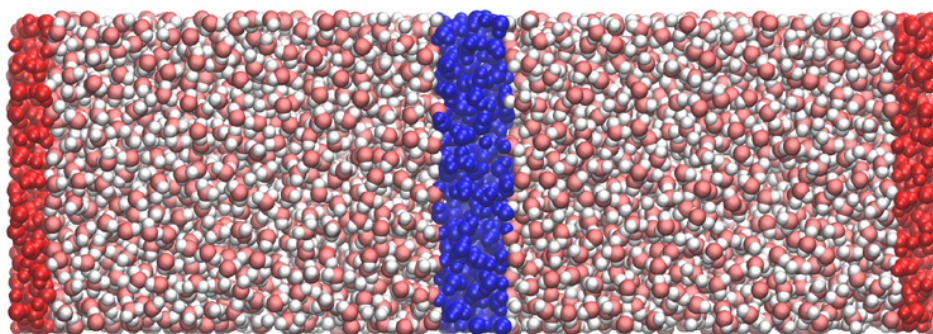


"An enhanced version of the heat exchange algorithm with excellent energy conservation properties"

by P. Wirnsberger, D. Frenkel and C. Dellago, *J. Chem. Phys.* **143**, 124104 (2015).

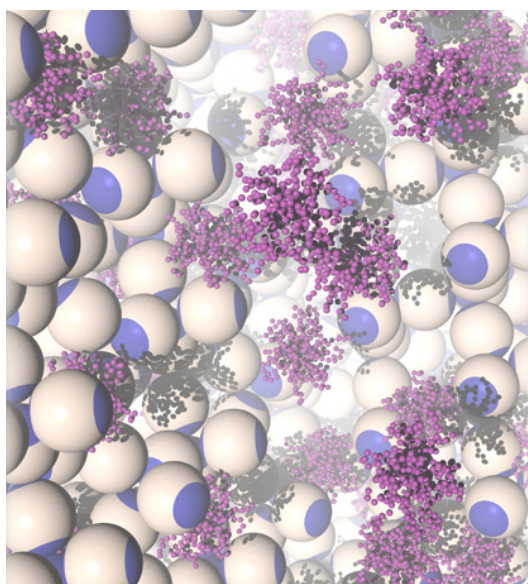
We have developed a new algorithm for non-equilibrium molecular dynamics simulations of thermal gradients. The algorithm is an extension of the heat exchange algorithm developed earlier by Hafskjold et al. in which a certain amount of heat is added to one region and removed from another by rescaling velocities appropriately. Since the amount of added and removed heat is the same and the dynamics between velocity rescaling steps is Hamiltonian, the heat exchange algorithm is expected

to conserve the energy. However, it has been reported previously that the original version of the heat exchange algorithm exhibits a pronounced drift in the total energy, the exact cause of which remained hitherto unclear. We have shown that the energy drift is due to the truncation error arising from the operator splitting and suggest an additional coordinate integration step as a remedy. The new algorithm retains all the advantages of the original one whilst exhibiting excellent energy conservation.



"Bottom-Up Colloidal Crystal Assembly with a Twist"

by N. A. Mahynski, L. Rovigatti, C. N. Likos and A. Z. Panagiotopoulos, *ACS Nano* **10**, 5459 (2016).



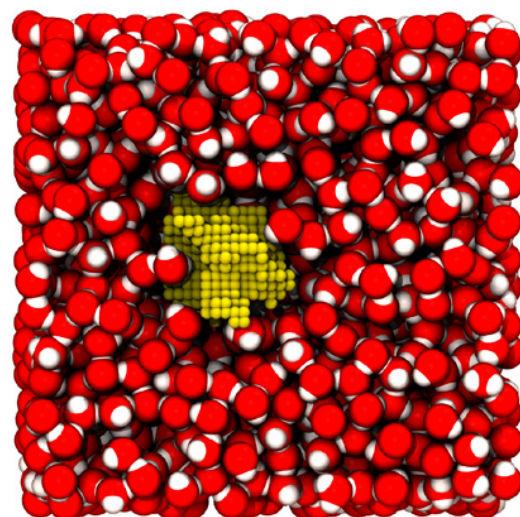
A cartoon of a mixture of spherical, rigid patchy colloids (white spheres with two blue patches on each pole) with soft, deformable star polymers, which act as structure-directing agents that selectively drive the self-assembly of the former into different structures.

In a paper published in the prestigious journal *ACS Nano*, former Lise-Meitner Fellow Lorenzo Rovigatti, working in the group of Christos Likos at the Faculty of Physics of the University of Vienna, in collaboration with Nathan Mahynski from NIST and Athanassios Panagiotopoulos from Princeton University (USA), has shown that long-range order can be restored by employing mixtures of colloids and polymer-based particles called star polymers. A cartoon of the system is sketched in the figure on the left. The former are designed to assemble into technologically relevant open crystals, which suffer, unfortunately, from the aforementioned polymorphism: the system crystallizes into a polymorphic mixture of a cubic and a hexagonal tetrastack crystal. However, the competing structures assembled by the colloids have different geometries and different internal void distributions. This difference can be exploited by tuning the star polymer size to interact uniquely with the void symmetry of the desired crystal, effectively stabilising it against the competitor. The research team employed sophisticated computer simulations to first evaluate the relative stability of the two polymorphs and then confirm the predicted effect by observing the complete transformation of a cubic tetrastack crystallite into a hexagonal one. The results of the research team serve not only to illustrate an alternative to existing approaches which, in many cases, produce unsatisfactory results, but also to guide experimental realizations of highly-ordered colloidal open crystals in the near future.

"Molecular mechanism for cavitation in water under tension"

by G. Menzl, M. A. Gonzalez, P. Geiger, F. Caupin, J. L. F. Abascal, C. Valeriani, C. Dellago, *Proc. Natl. Acad. Sci. USA* **113**, 13582 (2016).

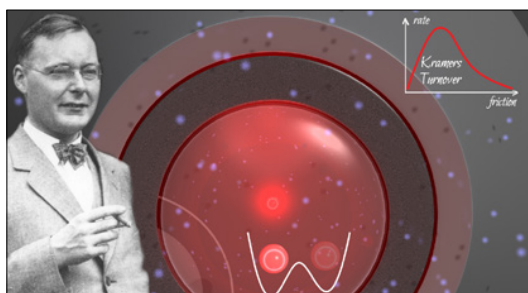
Cavitation, the formation of vapor-filled bubbles in a liquid at low pressures, is a powerful phenomenon with important consequences in nature and technology. For instance, cavitation bubbles may interrupt water flow in plants under dry conditions or severely damage the metal surfaces of machines such as pumps and propellers. In an international collaboration with scientists in France and Spain, we have used molecular simulations to study cavitation in water at strongly negative pressures and reveal its molecular mechanism. As reported in a recent paper in the prestigious *Proceedings of the National Academy of the USA*, we find that bubble growth is governed by the viscosity of the liquid. Although small bubbles are shaped irregularly, classical nucleation theory accurately describes the free energy barrier that impedes rapid bubble formation. Our simulations indicate that water can withstand negative pressures exceeding -120 MPa in agreement with recent experiments.



"Direct measurement of Kramers turnover with a levitated nanoparticle"

by L. Rondin, J. Gieseler, F. Ricci, R. Quidant, C. Dellago and L. Novotny, *Nature Nanotechnology* **12**, 1130 (2017).

Transitions occurring in nanoscale systems, such as a chemical reaction or the folding of a protein, are strongly affected by friction and thermal noise. Almost 80 years ago, the Dutch physicist Hendrik Kramers predicted that such transitions occur most frequently at intermediate friction, an effect known as Kramers turnover. In a team of scientists from the ETH Zurich, ICFO in Barcelona and the University of Vienna we have now measured and explained this effect for a laser-trapped particle, directly confirming Kramers' prediction in an experiment for the first time.

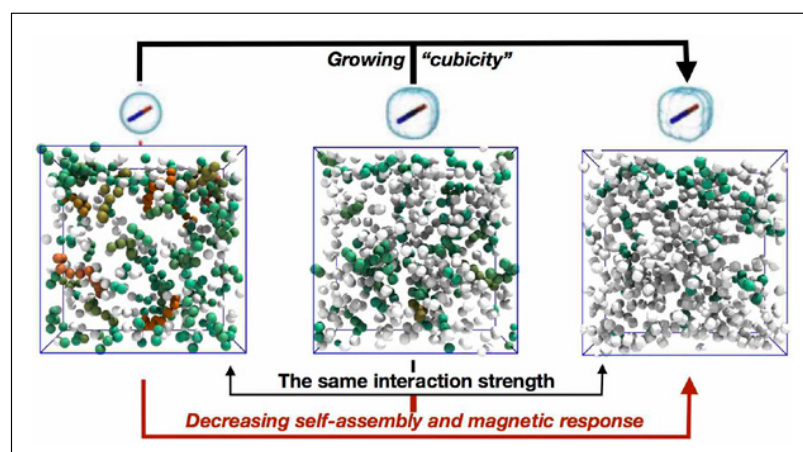


In 1940, Hendrik Kramers (left) predicted theoretically that in a double-well system (center bottom) transitions between the stable states happen most frequently at intermediate friction (upper right). The background shows a detail of the laser system used to confirm Kramers' prediction experimentally.

"Nanoparticle Shape Influences the Magnetic Response of Ferro-Colloids"

by J. G. Donaldson, E. S. Pyanzina and S. S. Kantorovich, *ACS Nano* **11**, 8153 (2017).

In a paper published in the prestigious journal *ACS Nano*, PhD student Joe Donaldson and visiting PostDoc Elena Pyanzina from the Ural Federal University have shown that in order to modify the magnetic response of conventional spherical magnetic colloids, the additional directionality can be conveniently introduced by considering systems composed of magnetic particles of different shapes. We presented a combined analytical and simulation study of permanently magnetized dipolar superball particles; a geometry that closely resembles magnetic cubes synthesized in experiments. We have focused on determining the initial magnetic susceptibility of these particles in dilute suspensions, seeking to quantify the effect of the superball shape parameter on the system response. In turn, we linked the computed susceptibilities to the system microstructure by analyzing cluster composition using a connectivity network analysis. Our study has shown that by increasing the shape parameter of these superball particles, one can alter the outcome of self-assembly processes, leading to the observation of an unanticipated decrease in the initial static magnetic susceptibility.



A cartoon showing how the shape affects the self-assembly of magnetic nanoparticles. The more cubic the particles, the lower is the effective self-assembly and the weaker is the magnetic response.

Dynamics of Condensed Systems

Mission Statement

The research group Dynamics of Condensed Systems is part of Key Research Area 4 (Complex Nanoscale Matter) of the Faculty of Physics. The group studies the properties of materials by scattering and spectroscopy techniques. The focus is on dynamics (diffusion and phonons) and kinetics of condensed systems. This includes metallic films, intermetallic alloys, oxide glasses, high entropy alloys, carbon nanophases, inorganic-organic hybrid systems, metallic and inorganic clusters and biomaterials such as bone tissue, feathers or hair.

More information can be found on our homepage: dcs.univie.ac.at

Research Highlights in the period 2015-2017

Diffusion of languages

Language shift is what happens when people switch from using one language to another. A question of particular interest is the motivation behind language shift: Why do people stop using one language and start using another? One way to try and answer this question are mathematical models. The process of language shift can be seen as a diffusion process similar to the process of physical diffusion (movement of atoms): a spread of the “new” language and resulting retreat of the “old” language, just like the spread of atoms. To study this spread of languages, a microscopic model for language diffusion was developed. The new model makes it possible to follow the evolution of language use in detail over time and space. It was tested using extensive empirical data on language shift in Carinthia, Austria (Slovenian to German). Using this example, it could be shown that the most important factor in determining the spread and retreat of a language is the interaction with speakers of the same language.

Reference:

K. Prochazka and G. Vogl: Quantifying the driving factors for language shift in a bilingual region;
Proc. Natl. Acad. Sci. USA 114 [17] (2017) 4365-4369, <http://dx.doi.org/10.1073/pnas.1617252114>.

Black phosphorous intercalation compounds

Black phosphorus is a 2D material with interesting properties such as a tunable band gap, high carrier mobility and strong interactions of light and matter. One approach to tune the properties is intercalation with alkali metals (namely: K and Na). Black phosphorous compounds (BPICs) have been synthesized in bulk by solid state as well as vapour phase reaction. By means of combination of in-situ XRD, Raman spectroscopy and DFT calculations, the structural behavior of the BPICs at different intercalation stages has been demonstrated for the first time. In Fig. 2, the splitting of the reflections in XRD was used to determine the development of the intercalated and the non-intercalated phase. Additionally, the growth of

K₃P and Na₃P compounds could be followed at higher alkali metal concentrations. These results provide a glimpse into the very first steps of a new family of intercalation compounds, with a distinct behavior with respect to its graphite analogues (GICs), showing a remarkably structural complexity and a dynamic behavior.

Reference:

G. Abellan, C. Neiss, V. Lloret, S. Wild, J.C. Chacon-Torres, K. Werbach, F. Fedi, H. Shiozawa, A. Görling, H. Peterlik, T. Pichler, F. Hauke, and A. Hirsch: Exploring the formation of black phosphorous intercalation compounds with alkali metals;
Angew. Chem. Int. Edit. 56 [48] (2017) 15267-15273, <http://dx.doi.org/10.1002/ange.201707462>.

Dynamics and chemical ordering in intermetallic alloys

A unique and new approach to study diffusion in solid materials on the atomic scale is given by the atomic-scale X-ray photon correlation spectroscopy. It is an extension of dynamic light scattering into the X-ray regime. By monitoring temporal intensity fluctuations of coherent speckles it allows to follow the dynamics at atomic length scales. Special emphasis must be given to the opportunity to measure atomistic diffusion at relatively low temperatures where such measurements were far out of reach with previously established methods. The importance of short-range order in a long-range ordered system has been demonstrated for the first time in a model B2-ordered Fe-Al system. We have shown in the paper that for long-range ordered systems the classical short-range order coefficients can be split into a term that depends only on the degree of long-range order and a fast decaying term that is due to real short-range order.

Reference:

M. Stana, B. Sepiol, R. Kozubski and M. Leitner: Chemical ordering beyond the superstructure in long-range ordered systems;
New J. Phys. 18 (2016) 113051, <http://dx.doi.org/10.1088/1367-2630/18/11/113051>.

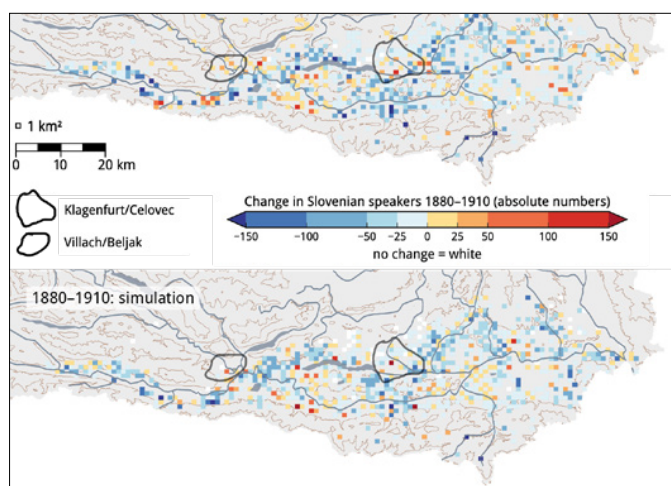


Fig. 1: Increase and decrease in the number of Slovenian speakers in southern Carinthia between 1880 and 1910. Top: Census data. Bottom: Optimum simulation. Source: PNAS 114(17): 4365.

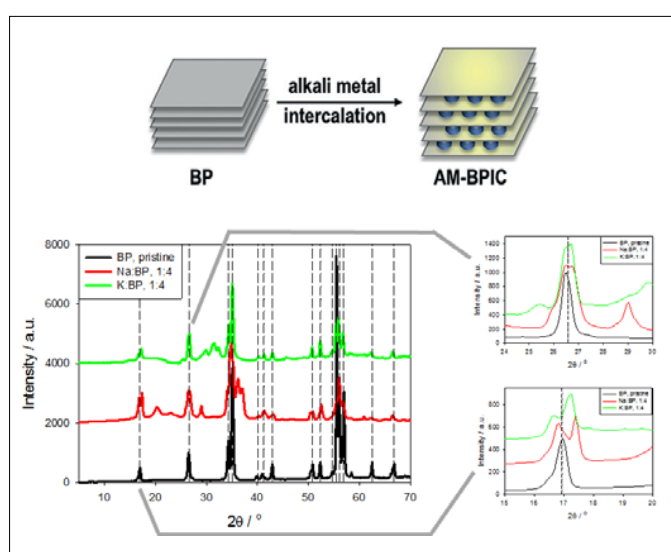


Fig. 2: Top: Principles of intercalation of black phosphorous with alkali metals. Bottom: Splitting of XRD peaks (enlarged in the right image) show the existence of an intercalated and a non-intercalated phase.

Further Selected Publications:

- P. Vecera et al. Precise determination of graphene functionalization by in-situ Raman spectroscopy. *Nature Communications* **8**, 15192 (2017).
- G. Abellan et al. Unifying principles of reductive covalent graphene functionalization. *JACS* **139**, 5175-5182 (2017).
- R. Belli et al. Chairside CAD/CAM materials. Part 1: Measurement of elastic constants and microstructural characterization. *Dental Materials* **33**, 84-98 (2017).
- P. Vecera et al. Solvent driven electron trapping and mass transport in reduced graphites to access perfect graphene. *Nature Communications* **7**, 12411 (2016).
- G. Rogl et al. Mechanical properties of half-Heusler alloys. *Acta Materialia* **107**, 178-195 (2016).
- T.A. Grünewald et al. Reaction of bone nanostructure to a biodegrading Magnesium WZ21 implant – A scanning small-angle X-ray scattering time study. *Acta Biomaterialia* **31**, 448-457 (2016).
- G. Rogl et al. In-doped multiferroic n-type skutterudites with ZT=1.8. *Acta Materialia* **95**, 201-211 (2015).
- D.S. Mahrhauser et al. Investigation of microemulsion microstructure and its impact on skin delivery of flufenamic acid. *International Journal of Pharmaceutics* **490**, 292-297 (2015).
- F. Essl et al. Biological Flora of the British Isles: *Ambrosia artemisiifolia*. *Journal of Ecology* **103**, 1069-1098 (2015).
- Z. Petrovic et al. Formation of RuO₂ nanoparticles by thermal decomposition of Ru(NO)(NO₃)₃. *Ceramics International* **41**, 7811-7815 (2015).

Electronic Properties of Materials

The research group EPM focuses on the experimental investigation of electronic properties of novel materials and condensed matter quantum systems. Archetypical examples of the correlated quantum solids are low dimensional carbon systems (fullerenes, carbon nano- tubes (CNT), and graphene), cuprate high-temperature superconductors, colossal magnetoresistance materials, and solar cells. Electronic properties denote physical quantities which are directly related to the response of the charge carriers on electric, magnetic, and electromagnetic fields. Our main goal is to unravel the correlated ground and excited state properties of these tailor-made low-dimensional systems in comparison with various state-of-the-art theoretical models to access their full application potential. The complex interplay between charge transfer, hybridisation, and charge transport is the key to their application potential and to designing novel materials with interesting electronic, optical and magnetic properties, such as one-dimensional metals or spin chains, two-dimensional devices based on the superconductors, carbon systems and solar cells.

Our group consists of three subgroups (Low Dimensional Quantum Solids, led by Thomas Pichler, Tailored Hybrid Systems, leader Paola Ayala, and Superconductivity, led by Wolfgang Lang). In addition to regular advanced teaching of PhD, master and bachelor students several group members are strongly involved in beginners' teaching (e.g. leading the beginners laboratory course (Wilhelm Markovitsch), teaching Experimental Physics 4 and the related exercise course (co-led by Thomas Pichler), and the Laboratory course Environmental Physics (co-led by Viktor Schlosser)). Thomas Pichler is also Vice-PhD Study dean for Natural Sciences and deputy head of the Vienna Doctoral School in Physics. Paola Ayala is the Gender and Equality representative of our Faculty.

2015-2017 we had 57 publications in peer-reviewed journals, including highlights in one *Physical Review Letters*, three *Scientific Reports*, one *ACS Nano*, one *Applied Physics Letters*, one *Chemistry of Materials*, one *Nano-scale*, one *Advanced Materials*, one *Advanced Functional Materials*, one *Nature Materials*, one *Nature Communications*, one *Angewandte Chemie*, one *Nano Letters*, one *2D Materials*, three *Carbon*, four *Physical Review B* and one *Physical Review Materials*. Two PhD students (Lei Shi, Nikolay Verbitskiy) finished in 2015 and 2016 on "Synthesis and Raman analysis of carbon chains inside double walled carbon nanotubes" and on "Synthesis and electronic properties of functionalized graphene on transparent substrates". Major outcomes were published in 2015 and 2016 in *Nature Materials and Advanced Functional Materials* [14, 15] and in *Scientific Reports and 2D Materials* [10,16]. In addition we had 60 invited presentations at international conferences, universities and research institutions. Our group co-organized the IWEPM conference series in Kirchberg (Tirol) (Hans Kuzmany) and organized the biggest conference on nanotubes in 2016, the NT16 conference with more than 430 attendees in Vienna (Paola Ayala). In 2017 Paola Ayala received by President Rafael Correa directly the highest research prize of Ecuador, the Matilde Hidalgo Prize for best scientist.

Selected Research Highlights

Superconductor/Ferromagnet bilayer structures

According to standard textbooks superconductivity and ferromagnetism are two mutually exclusive macroscopic quantum phenomena. Intriguingly, in few-nm-thick bilayer films consisting of thin sheets of the metallic superconductor NbTiN and the weak ferromagnet NiCu, the superconducting effect can even extend into the ferromagnetic layer by the proximity effect. Such systems are interesting for superconducting single-photon detectors. One of the key figures of merit of such detectors is a low dark-count rate, i. e., a spurious read-out without photon incidence that is connected to thermodynamic fluctuations of the superconducting order parameter. In an international collaboration we have started to measure these fluctuations via paraconductivity and magnetoresistance and analyze them within the available theoretical background. Fluctuations are significantly suppressed in the bilayers, making them promising candidates for enhanced single-photon detectors.

Low dimensional quantum solids & tailored hybrid systems

We made great progress in understanding the complex influence of environmental effects as well as controlled functionalization in nanotubes and graphene. This was performed either via in-situ doping by substitutional phosphorous during single walled carbon nanotubes synthesis [1] or by post functionalization via advanced filling reactions [2, 21] followed by nanochemical reactions [6] and upon electrochemical doping [3]. We theoretically analyzed the details in the core level binding energy [8], unraveled the dopant-configuration controlled carrier scattering in graphene [9] and achieved an atomically precise control of the graphene/h-BN interface to classical semiconductors by Ge intercalation [10]. For doping of nanotubes and graphene by intercalation, we contributed to the understand-

ing of the doping of multi walled nanotubes [17], used doped nanotubes as model systems for graphene [24], unraveled all stable phases in the alkali metal intercalation of black phosphorous [26] as well as showed how to achieve a control of the electron-phonon interaction in Ba doped graphene via the environment [13]. The reaction of intercalated graphite also allowed to achieve control over the functionalization degree in graphene [22]. We also made progress for pristine nanotubes in the controlled isotope arrangement in ^{13}C enriched carbon nanotubes [19] and in understanding how vacancy oxidation influences the properties of metallicity sorted carbon nanotubes [28]. As a new material we were able to produce confined carbene chains inside double walled carbon nanotubes [15], understand their length dependent Raman response [18], filling dependent enhancement of the photoluminescence of the inner tubes [16] and reveal the energy gap of the confined chains as function of length and environment via resonance Raman spectroscopy [27]. We also had new pioneering developments regarding in-situ Raman spectroscopy [22] and an optically detected magnetic resonance spectrometer with tunable laser excitation and wavelength resolved infrared detection [20].

In addition, we contributed to determine their and MoS_2 applications in oxygen reduction [5,11] and as chemsensors and supercapacitors [4,7,12]. We also had important new results regarding microscale magnetic compasses [25] and the doping of metal-organic frameworks towards resistive sensing [23].

Highlighting five of these results we have for the first time been able to effectively tune the localized transverse surface plasmon resonance in metallicity sorted nanotubes upon ionic liquid electrochemical doping [3]. In close cooperation with Kazu Suenaga at AIST we were able to use modern high resolution electron energy loss spectroscopy to directly correlate the local structure of single walled carbon nanotubes to their electronic transport and optical properties. This can be seen as a breakthrough as it allows

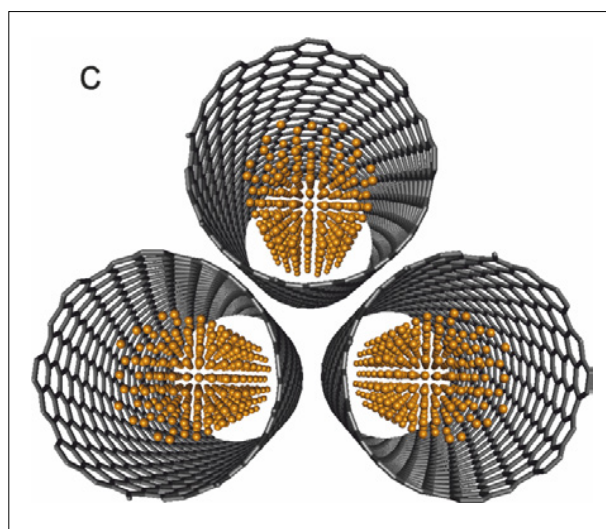


Fig. 1: Schematic of fcc nickel clusters encapsulated in bundled SWCNTs. Figure adapted from Ref. [6].

for the first time to for instance directly access the extension of excitons and to study the charge localization at defects as well as to identify the effective core hole contribution in the C1s core hole excitation fine structure using different individual nanotubes as benchmark [14]. Regarding filled nanotubes we have synthesized ensembles of fcc nickel nanowires with defined mean sizes in the interior of single-wall carbon nanotubes [6] (see Fig. 1). The method allows the intrinsic nature of single-domain magnets to emerge with large coercivity as their size becomes as small as the exchange length of nickel. Recently as a third highlight we made significant progress towards accessing the application potential of graphene in nanoelectronics and regarding the integration into classical semiconductor technology [10]. So far these applications are limited by the ability to concomitantly achieve large single-crystalline domains on dielectrics and semiconductors and to tailor the interfaces between them with an atomistic precision. We showed a new direct bottom-up method for the fabrication of high-quality atomically precise interfaces between 2D materials, like graphene and hexagonal boron nitride (hBN), and classical semiconductor via Ge intercalation. Using angle-resolved photoemission spectroscopy (ARPES) and complementary DFT modelling we observed for the first time that epitaxially grown

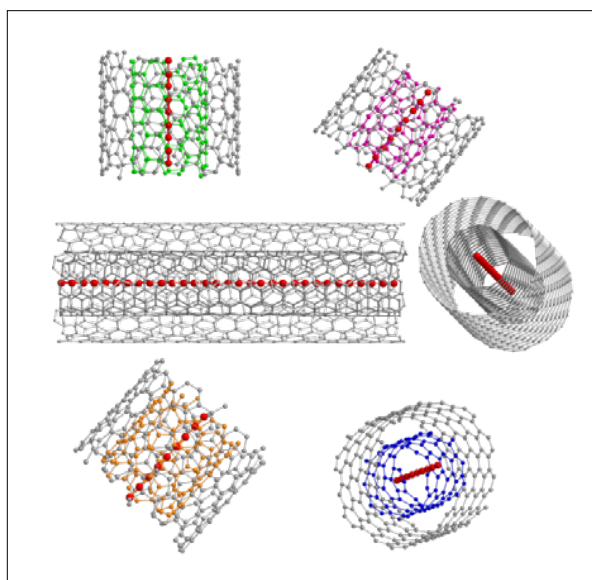


Fig. 2: Schematic representation of confined ultra-long acetylenic linear carbon chains inside different double walled carbon nanotubes.

graphene with the Ge monolayer underneath demonstrates Dirac fermions unaffected by the substrate as well as an unperturbed electronic band structure of hBN. This approach provides the intrinsic relativistic 2D electron gas towards integration in semiconductor technology [10].

In 2016 we had for the first time stabilized confined carbyne as last missing allotrope of carbon. Even in its elemental form, the high bond versatility of carbon allows for many different well-known materials, including diamond and graphite, graphene and fullerenes. Although the existence of carbyne, an infinitely long one-dimensional carbon chain, was proposed in 1885 by Adolf von Baeyer (Nobel laureate for his overall contributions in organic chemistry, 1905), scientists have not yet been able to synthesize this material as last missing carbon allotrope. Von Baeyer even suggested that carbyne would remain elusive as its high reactivity would always lead to its immediate destruction. Nevertheless, carbon chains of increasing length have been successfully synthesized over the last 50 years, with a record of around 100 carbon atoms (2003). This record has now been broken by more than one order of magnitude, with

the demonstration of micrometer length-scale chains [15].

We have therefore succeeded in developing a novel route for the bulk production of ultra long carbon chains composed of more than 6,000 carbon atoms, using thin double-walled carbon nanotubes as protective hosts for the chains (see sketch in Fig. 2).

These findings represent an elegant forerunner towards the final goal of carbyne's bulk production and are the first proof of confined carbyne [15]. The direct experimental proof of confined ultra-long linear carbon chains, which are more than an order of magnitude longer than the longest proven chains so far, can be seen as a promising step towards the final goal of unraveling the intrinsic properties of the last missing carbon allotrope, carbyne. Regarding application, carbyne is very stable inside double-walled carbon nanotubes. This property is crucial for its eventual application in future materials and devices. According to theoretical models, carbyne's mechanical properties exceed all known materials, outperforming both graphene and diamond. Carbyne's electrical properties suggest novel nanoelectronic applications in quantum spin transport and magnetic semiconductors as has been recently revealed by measuring its energy gap.

As a last highlight we had an important contribution in unraveling the properties of covalently functionalized graphene using a specific setup developed in our group allowing a new form of in-situ Raman spectroscopy [22]. This is of crucial importance as graphene is considered as one of the most promising new materials. However, a successful use of graphene in the semiconductor industry can only be achieved if properties such as the conductivity, the size and the defects of the graphene structure induced by the functional groups can already be modulated during the synthesis of graphene. This systematic insertion of chemically bound atoms and molecules to control its properties is still a major challenge. Now, for the first time, in close

cooperation with the organic chemistry group led by A. Hirsch in Erlangen we succeeded in precisely verifying not only the type but also the functionalization degree with covalent groups of graphene based compounds [22]. A schematic representation is shown in Fig. 3.

These unique properties offer a wide range of future applications as e.g. for new developments in optoelectronics or ultrafast components in the semiconductor industry. As mentioned above, we accomplished a crucial breakthrough: using our abovementioned newly developed experimental set-up we were able to identify, for the first time, vibrational spectra as the specific fingerprints of step-by-step chemically modified graphene by means of light scattering. This spectral signature, which was also theoretically attested, allows determining the type and the number of functional groups in a fast and precise way. Among the reactions we examined, was the chemical binding of hydrogen to graphene. This was implemented by a controlled chemical reaction between water and particular compounds in which ions are inserted in graphite, a crystalline form of carbon [22].

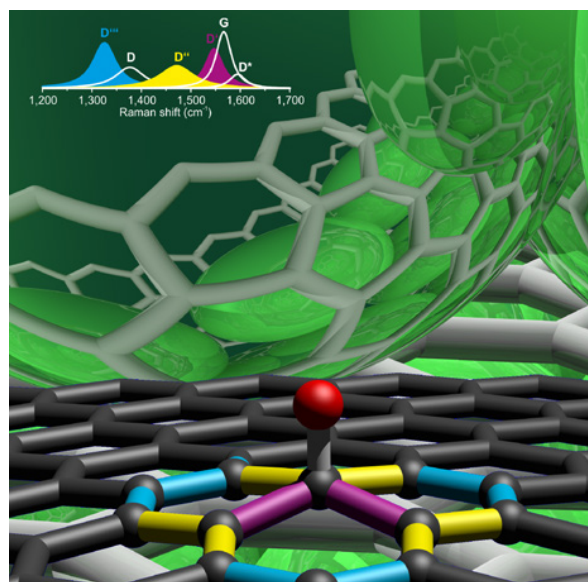


Fig. 3: Section of a graphene network with chemically bound hydrogen atom: the spectral vibrational signature of the single carbon-carbon bonds adjacent to the bound hydrogen atom is highlighted in different colors.

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Faculty Center for Nano Structure Research

Mission Statement

The Faculty Center for Nano Structure Research is an institutional cooperation between the Faculties of Physics and Chemistry. It is located at the Faculty of Physics and offers scientists and students of the two faculties an easy access to large and expensive instruments, among them the Zeiss Supra 55 VP environmental scanning electron microscope, the WITec alpha 300A atomic force microscope / Raman and the Bruker Nanostar laboratory small-angle X-ray system. All are usually fully booked at least one week in advance and have an average utilization of above 95 %. Other services offered include, but are not limited to, sample mounting, grinding, optical microscopy, fluorescence microscopy, sample etching, sputter coating, microhardness measurements and the determination of elastic constants as a function of temperature.

Summary

An investment grant from the Faculty of Physics made it possible to replace the aging Anton Paar MTH-4 microhardness tester, which was directly mounted on a Zeiss Axioplan materials science optical microscope, with a new system, again by Anton Paar. The new machine, a CSM Micro, is a stand-alone microhardness tester, built around a stiff frame. The possible load ranges from 0.01 to 30 N and both the measurement of the depth-load curve and of the size and depth of the imprint can be done fully automated. The sample hardness can both be measured along a line with a predefined spacing or at every point of a grid. The system is available to the members of the faculties as of January 1st 2016. Prospective users are requested to contact Martina Rohrer for an appointment.

Additionally, the Faculty Center received a fluorescence microscope as a loan from the quantum optics group. All standard microscopy techniques – from transmitted light bright-field to epi-fluorescence – can be used without any restrictions. The light source in the reflected light mode is a HBO 100 mercury vapor lamp, with an upstream Schott-glass optics, which results in a lower cut-off wavelength of the UV spectrum at 344 nm. The light source in the transmitted light mode is a white Thorlabs LED. Several object lenses and filters are available. Fluorescence images can be acquired with an Andor iXon3 high sensitivity EMCCD camera, which is attached to the microscope. Prospective users are requested to contact Christian Knobloch for an appointment.

Financial support from the Faculty of Chemistry and the Faculty of Physics made it possible to acquire a WITec alpha 300A. It is a high-resolution combined atomic force microscope / Raman system for the non-destructive characterization of nanostructures. The confocal Raman system allows for spectroscopic measurements of molecules and solids with high spectral and lateral resolution while the integrated atomic force module (AFM) can be used for the topographic characterization of surfaces with nano-scale precision. Using the combination of both techniques, the WITec alpha 300A can also perform correlated measurements of AFM and Raman and is an all-purpose microscope for nanoanalytics. The system was available to the members of the faculties as of January 1st 2017. Prospective users are requested to contact Dieter Baurecht from the Faculty of Chemistry for an appointment.

More information can be found on our homepage: nanozentrum.univie.ac.at

An overview of the research done at the Faculty Center in 2015-2017

Research at the Faculty Center is almost always initiated by other groups in the Faculties of Physics and Chemistry. After an initial training period, the experiments are performed predominantly by members of those groups. What follows are examples of research that was done, at least partly, on equipment provided by the center or research done by staff members.

Quantum Physics

Optical cavities using Bragg mirrors can be used in a variety of ways, like extremely high resolution molecular IR spectroscopy, but even the best mirrors contain a number of defects. In order to optimize the production of those mirrors and to minimize the number of defects, it is necessary to investigate their genesis. Especially the topography of a defect allows insights into its formation.

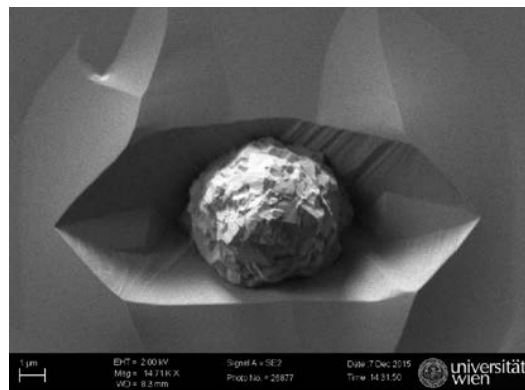


Fig. 1: A partly overgrown defect in a Bragg mirror manufactured by Crystalline Mirror Solutions.

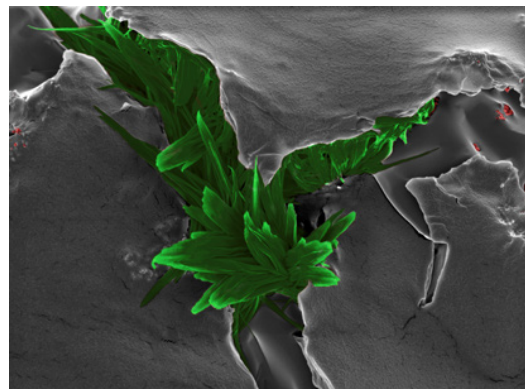


Fig. 2: Pluronic F-127 entities (colored green) growing out of the polymer upon drying. Only a few nanoparticles are visible (colored red) in the fissures.

Biological Chemistry

M. Hafner, from the group of C. Becker, Institute of Biological Chemistry, investigated nanoparticles, which are enclosed by a lipid-layer, which in turn is created from a compound of oleic acid and Pluronic F-127. Pluronic F-127 is a copolymer whose role is to increase the viscosity of the solution in order to replicate the cytoplasm of a natural cell.

Material Chemistry [1]

I. Jandl, from the group of K. Richter, Institute of Materials Chemistry, investigated the ternary Ni-Pd-Sn system from 700 °C upwards. Special focus was put on the B8-type phase. Cast samples (see Fig. 3) were examined and a liquidus surface projection was constructed for the entire ternary system based on a combination of the experimental and literature data.

Biological Chemistry [2]

The Tanpopo orbital mission performs a long-term outer space exposure of the multiple extremes resistant bacterium *Deinococcus radiodurans* aiming to investigate the possibility of interplanetary transfer of life. The aim of this study was to decipher the molecular response of *D. radiodurans* to space-related conditions of UVC radiation and vacuum prior to the space mission and using the experimental set-up of the Tanpopo orbital project. Scanning electron microscopy investigations showed that neither morphology nor cellular integrity of irradiated cells were affected, while integrated proteomic and metabolomic analysis revealed numerous molecular alterations in metabolic and stress response pathways. Several molecular key mechanisms of *D. radiodurans*, including the tri-carboxylic acid cycle, the DNA damage response systems, ROS scavenging systems and transcriptional regulators responded in order to cope with the stressful situation caused by UVC irradiation under vacuum conditions.

Material Physics [3]

The Faculty Center contributed, in a cooperation with the University of Erlangen-Nürnberg, with X-ray structural analysis to the development of a scalable and inexpensive method for graphene production surpassing previous wet-chemical approaches. This could be realized by simple treatment of dispersed graphenides suspended on silica substrates with benzonitrile, which leads to a clean conversion to graphene.

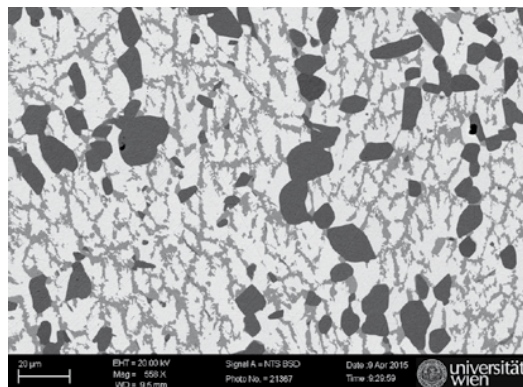


Fig. 3: Backscattered electron image of a Ni40Pd30Sn30 sample. The light-colored regions are the B8-phase.

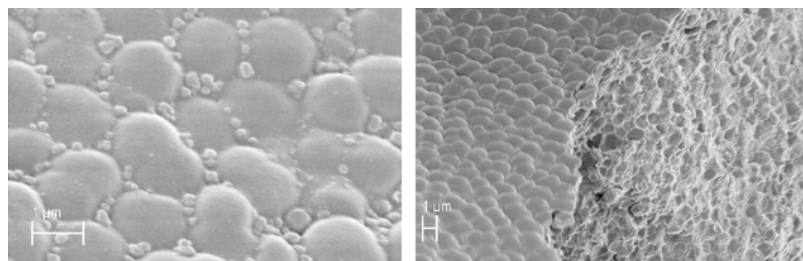


Fig. 4: Scanning electron microscopy images of the upper surface of dehydrated *D. radiodurans* deposited on aluminum plates.

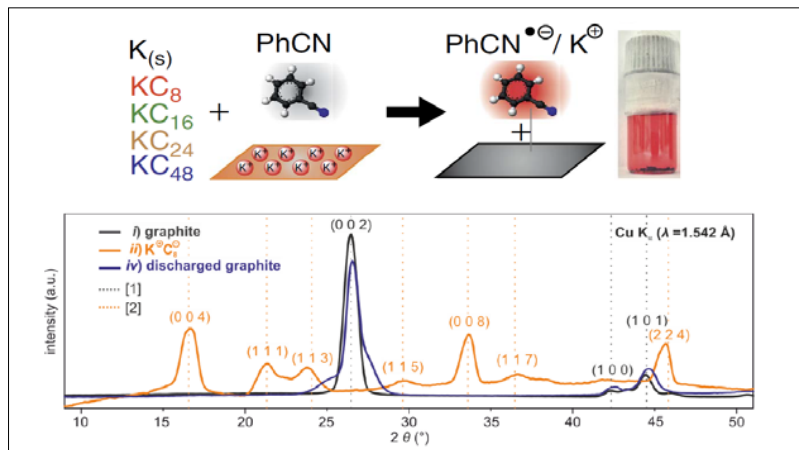


Fig. 5: Top: Reaction scheme for the quantitative electron transfer from various GICs to PhCN, together with a photo of a sealed vial containing KC8 in PhCN. Bottom: XRD patterns of charged and discharged graphite.

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Gravitational Physics

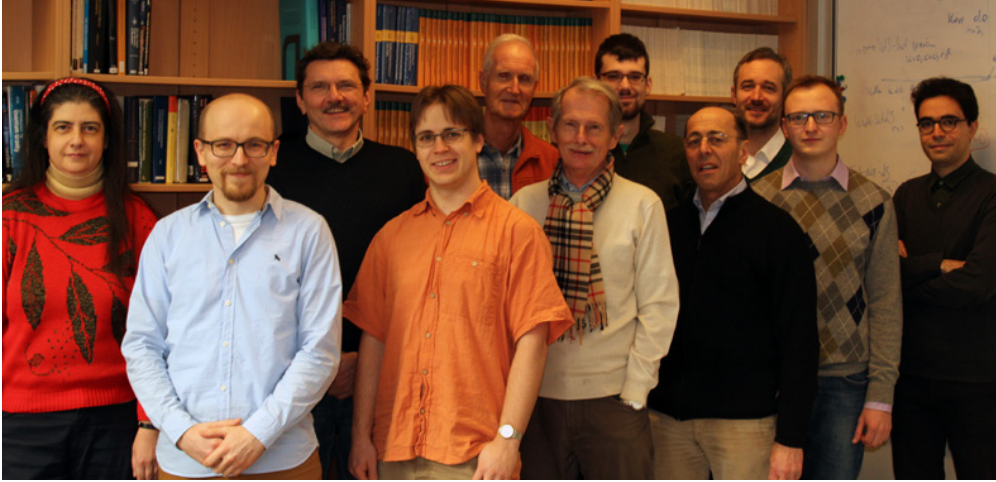


Fig. 1: Some students and members of the gravitational physics group.

The group

The main focus of research of the gravitational physics group is mathematical general relativity, with the aim of understanding the many aspects of the global structure of spacetimes. This includes studies of formation of singularities and their properties, the understanding of the long term behaviour of gravitating systems, as well as various aspects of the Cauchy problem in general relativity. The latter includes questions such as black hole formation and stability, or construction of initial data with significant physical properties, with data on spacelike hypersurfaces or on characteristic ones. Another direction of our studies are the various facets of black holes, including uniqueness and existence theorems, formation of trapped surfaces, or inequalities relating global geometric invariants. Models with matter are also of interest: the group has been very successful in recent studies of self-gravitating ensembles of collisionless particles, known as the Einstein-Maxwell model. Yet another direction of research is the study of self-gravitating (Newtonian and relativistic) elastic matter models, which have been largely unexplored so far and are bound to play an important role in astrophysics. Here, as well as in other problems raised above, even those configurations which are small deformations of equilibria pose formidable mathematical challenges.

In addition to these main topics, members of our group keep an active interest in questions such as instantons in Euclidean quantum gravity, singularity avoidance in effective quantum gravity for simple collapse scenarios, or the problem of trans-Planckian frequencies in black hole evaporation. We also have an eye out on waveguide experiments testing special relativity or weak gravitational fields.

The scientific context

The last three years have been wonder years for gravitational physics. After a major instrumental rehaul, the Laser Interferometric Gravitational Observatory (LIGO) has started taking data in the fall of 2015, making the first direct observation of gravitational waves within the first few days of operation. This achievement has been rewarded by a Nobel Prize in 2017. Six more detections have been announced since. In addition to the first breakthrough observation, the two most notable ones are the first three-instrument detection of a gravitational wave by the LIGO observatory jointly with the European VIRGO observatory, which went online in an upgraded configuration in the summer of 2017. The third notable event was the first multi-messenger detection of a merger of two neutron stars, again in the summer of 2017. In addition to the gravitational waves, the stellar collision has been seen and studied in all electromagnetic bands (X rays, radio waves, optical) by some seventy instruments on earth and on satellites. In addition to providing a direct observation of gravitational waves, the detections established existence of a large population of black holes with an unexpected range of masses, and provided direct observational evidence of existence of binary systems of black holes.

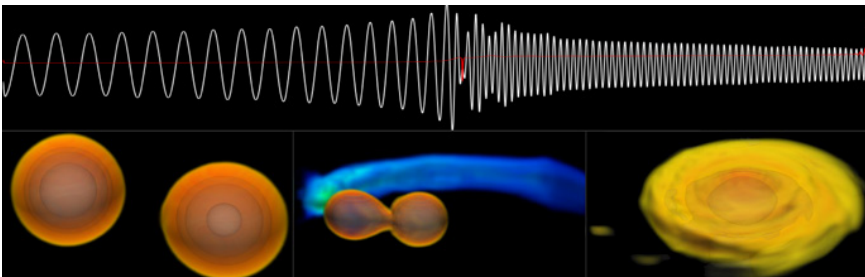


Fig. 2: Gravitational waves from the collapse of an equal-mass neutron star merger.

News

The detection of gravitational waves and the Nobel Prize in Physics 2017 has seen a flurry of public talks, colloquium talks, and conferences on the topic. Peter Aichelburg, Piotr Chruściel and Helmut Rumpf have been invited to speak at many such events, including prestigious conferences in London and Stockholm.

David Fajman, who has been a postdoc in the group so far, has been ranked first in a very competitive field of applicants for a tenure track position at our Faculty of Physics. He will start his appointment in January 2018. His position was filled in September 2017 by Maciej Maliborski, previously Humboldt Fellow at the Albert Einstein Institute in Potsdam.

Jérémie Joudioux has left the group to lecture at the University of Nijmegen. We regret that we couldn't keep him in the group, and wish him a very successful future career. His position will be filled by Stefan Palenta, a fresh PhD graduate from Jena, in January 2018.

Peter Aichelburg has continued his excellent work as our outreach ambassador, giving public lectures at the Kinderuni Wien, at the Universities of Vienna and Leoben, at the Alpbach Forum, and others.

Research Highlights

Periodic solutions of wave equations are notoriously difficult to construct, and this is especially so in general relativity. It therefore came as a surprise when Piotr Chruściel discovered a new class of time-periodic solutions of Einstein equations with a negative cosmological constant, and proved their existence (arXiv preprint 1711.11261). The intriguing existence argument appeals to seemingly unrelated tools of the theory of elliptic partial differential equations and complex analysis. The proof is flexible enough to establish the existence of periodic solutions of a wide class of wave equations, not only the Einstein ones.

In every physical theory an important role is played by stationary solutions. In a series of papers in collaboration with Erwann Delay (Avignon) and PhD student Paul Klinger, Piotr Chruściel has proved existence of large new classes of such solutions for Einstein equations with a negative cosmological constant and with various matter fields. The solutions comprise globally stationary solutions, as well as time-independent black holes. The above authors were pleased to collaborate in one of their papers with Andreas Kriegel, Peter Michor, and Armin Rainer, all from the Vienna Faculty of Mathematics, in the construction of a new class of boson stars.

An unexpected feature of Einstein equations, discovered by Carlotto and Schoen in 2014, is the possibility to shield-away the gravitational

field using the gravitation field. (What is most surprising is that something like that is not possible in Newtonian gravity.) Piotr Chruściel with collaborators has been actively developing this direction of research. Together with Erwann Delay they refined and generalized various aspects of the Carlotto-Schoen construction. Together with Beig they showed how to carry out the shielding in linearized Einstein gravity by completely elementary methods.

One of the mainstream directions in mathematical general relativity is the study of existence, stability, and global dynamical properties of solutions of Einstein equations. In a breakthrough paper (arXiv:1707.06141), David Fajman, Jérémie Joudioux and Jacques Smulevici (Paris-Orsay) have proved global existence of a large class of solutions of the Einstein equations coupled to the Vlasov matter fields, with initial data near those for Minkowski space-time. In this model objects such as galaxies are described as a gas of particles interacting gravitationally. The proof builds upon their previously published studies (Analysis and PDE, Vol. 10 2017) of the asymptotic behaviour of the Vlasov-Nordström system of equations.

Another core question in general relativity is the classification of regular black hole solutions. A generalization of the Weyl tensor, the so-called Mars-Simon tensor (MST), was introduced to provide a characterization of the Kerr family of black holes, and its generalization to include a cosmological constant. In joint work with M. Mars (Salamanca) and J. Senovilla (Bilbao), T. Paetz and W. Simon characterized asymptotic Cauchy data on a spacelike boundary at infinity which generate vacuum spacetimes with vanishing MST, leading to a new classification of these spacetimes.

A thorough understanding of self-gravitating elastic bodies is critical for a proper treatment of e.g. neutron stars, and it is clear that such models will play an ever-increasing role in astrophysics. A few years back, Robert Beig and collaborators initiated the study of such systems in a general relativistic context, and have since been systematically analysing all the facets of the problem. In the reporting years Beig and Schmidt established existence of low-regularity-solutions to the field equations describing the motion of compact, gravitating elastic bodies in full general relativity. A challenging current problem is to extend these solutions to regular solutions.

Isotope Research and Nuclear Physics

Mission

We focus on the applications and on the physics to measure extremely small amounts of long-lived radioisotopes such as ^{10}Be , ^{14}C , ^{26}Al , ^{36}Cl , ^{41}Ca , ^{129}I , ^{182}Hf , the actinides and fission fragments. Due to their finite lifetime most of those radioisotopes should be extinct by now, but natural or man-made processes produce them in minute quantities. Thus, they allow studying phenomena in many domains of nature, from archeological dating to supernova remnants. Technical and methodological developments center on the Vienna Environmental Research Accelerator (VERA) to provide world-class capabilities for accelerator mass spectrometry (AMS). The purpose of our 3 MV Tandem accelerator is to eliminate molecular interferences in mass spectrometry and to provide sufficient energy in the MeV range to help identify every ion by its nuclear charge. We mainly pursue AMS measurements related to archeology, geophysics, astrophysics, as well as experimental work related to neutron-induced reactions and to environmental radioactivity.

Dating and tracing applications with ^{10}Be , ^{14}C , ^{129}I

Many of our accomplishments in the particularly important field of radiocarbon dating are part of well-established collaborations, e.g. the long-standing cooperation with Sturt Manning (Cornell University, USA) with a focus on samples from ancient Middle East, see e.g. [1], or with João Zilhão (Universitat de Barcelona) on *Homo neanderthalensis*, see e.g. [2]. We also collaborate with Anna Łosiak, Polish Academy of Sciences, on dating the Kaali Impact Crater (Estonia) [3].

The article “Altersbestimmung dank Atomtests” in *Spektrum der Wissenschaft*, 62, März (2016) by E. M. Wild and W. Kutschera was well-received by the public.

Carrier-free $^{10}\text{Be}/^9\text{Be}$ measurements became routinely available at VERA in 2015. The method was successfully applied to measure accumulation rates of slowly growing ferromanganese crusts.

For example, these archives record isotope signatures of past supernova explosions in the Earth's vicinity (see astrophysics).

Within the Vienna Environmental Sciences Research Network we started collaborating with the Department of Geography and Regional Research on studying the meltdown of ice lenses in the Kaunertal (Tirol) and their effect on the Alpine erosion. Our detection capabilities of anthropogenic ^{129}I in water samples allow for age determination of the melt water and of the ice.

An exciting possibility to date ceramics by controlled water uptake, the so-called rehydroxylation (RHX) method, was published by a British group in 2009. We have performed a thorough investigation of background problems with this method, and like several other groups, could not verify the original claim.

Actinides

Several projects utilize the outstanding capabilities of VERA to measure extremely low amounts of actinides.

Final results for a uranium metal cube originating from the German World-War II experimental nuclear reactor “B8” at Heigerloch were achieved by an international collaboration. AMS measurements of ^{236}U proved that the unit was never critical [5].

We succeeded in obtaining the first depth profile of ^{236}U for a sampling station in the Northeast Pacific Ocean using only one liter of seawater sample from each depth. ^{236}U concentrations showed large variations between ca. 10^7 atoms/kg at 60 m depth and ca. 10^5 atoms/kg at 3000 m depth.

Together with colleagues from TU Munich in Germany we could also demonstrate by AMS that no effects of the Fukushima accident are observed for plutonium isotopes $^{239-241}\text{Pu}$ dissolved in Pacific ocean water.

Nuclear physics and astrophysics

A certain amount of ^{244}Pu from recent supernova explosions was expected by theory to be found in the solar system. However, in practice it could not be detected in deep-sea reservoirs all across the globe. The production of ^{244}Pu , the heaviest long-lived radionuclide with a half-life of 81 Ma, is a sensitive indicator of explosive nucleosynthesis at extreme neutron densities. A collaboration between VERA, TU Munich, Hebrew University in Israel, and ANU in Canberra, Australia, measured ^{244}Pu in deep-sea sediments, resulting in a first indication that rare neutron-star mergers may have predominantly created this neutron-rich nuclide in our galaxy, and not the more frequent supernovae. The result was published in *Nature Communications* [5].

A long-standing discrepancy about the half-life of ^{60}Fe (2.6 Myr), an important astrophysical chronometer, could be settled by a collaborative effort of scientists from VERA, the Atominstitut in Vienna, PSI in Switzerland, and ANU, Australia. The result was published in *Physical Review Letters* [7].

Walter Kutschera, together with Gunther Korschinek from the TU Munich, wrote a comprehensive review about searches for super-heavy elements in nature [8].

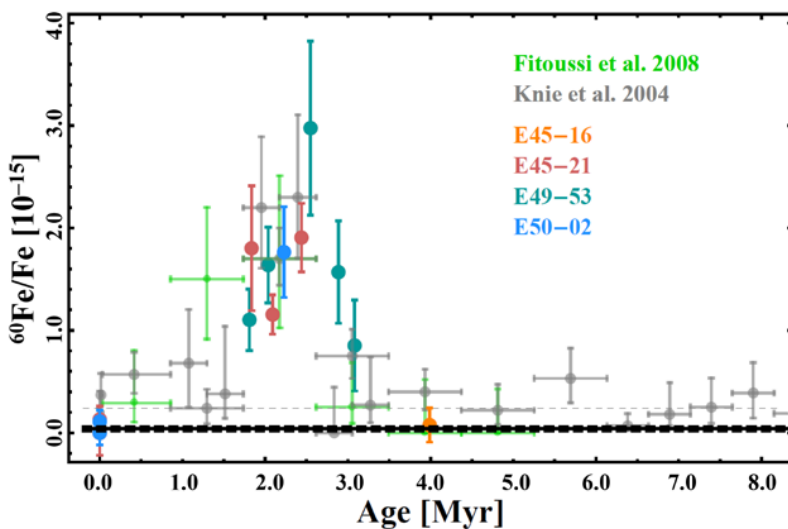
Within the n_TOF collaboration at the European Laboratory for Particle Physics (CERN), we study neutron induced nuclear reactions relevant for astrophysical processes in stars and in supernovae as well as for possible advanced nuclear fuel cycles. The n_TOF facility, located in an underground tunnel at CERN, consists of a pulsed spallation neutron source and two neutron time-of-flight spectrometers. The much higher neutron fluence of the newly operating "short" flight path (19 m) enables us to measure smaller reaction cross sections and use smaller samples, e.g. for (n,α) reactions on light nuclei in the neutron energy range 3 to 15 MeV. Such data are required for technical and also for biological applications.

Natural radioactivity

Our activities concerning natural radiation concentrated on two projects:

In an ongoing investigation we study the influence of geological parameters on the indoor radon concentration. Systematic measurements of radon concentration in soil gas, permeability of the soil, uranium, thorium and radium concentration in soil, ambient dose rates and indoor radon concentrations in several municipalities in Styria were performed and analyzed for correlations, see e.g. [9].

The second project deals with the reuse of residues and wastes which contain enhanced concentrations of natural radionuclides (NORM). Enormous amounts of e.g. phosphogypsum, red mud, slack from iron and other metal production, sludge from the oil industry are presently disposed in the environment. The COST action NORM4BUILDING aims to use such residues in building material to reduce the negative environmental effects of disposal areas, to supply the building industry with high quality raw materials and to ensure radiation safety for producers and users of such products.



The figure shows the abundance of the radionuclide ^{60}Fe (half-life 2.6 Myr) as function of age in various archives; the deep-sea sediments from this work are labelled by En-m. An enhancement at 1.7 – 3.2 Myr is due to supernova explosions and massive star events; for details see A. Wallner et al., *Nature* 532, 69–72 (2016).

Another highlight was the report in *Nature* [6] that the ^{60}Fe signal observed previously in deep-sea crusts is of global character, is extended in time and is of interstellar origin from multiple events. Deep-sea archives from all major oceans were analyzed for ^{60}Fe deposition. Our results reveal ^{60}Fe interstellar influxes onto Earth 1.7–3.2 Myr ago, see figure. The measured signal implies that a few percent of fresh ^{60}Fe was captured in dust and deposited on Earth. Our findings indicate multiple supernova and massive-star events during the last ~10 Myr at nearby distances ≤ 100 parsec.

Cooling and photo-detachment of negatively charged ions

After years of development the “Ion-Laser Inter-Action AMS” (ILIAMS) reached first spectacular results [10]. Our aim is a principally new approach for isobar suppression in AMS, i.e. by element-selective elimination of unwanted negative ions before the accelerator. Key of this method is the photo-detachment of the interfering isobars at sub-eV kinetic energy in a linear, gas-filled radio-frequency quadrupole by a suitable laser. The anions of interest remain unaffected by the laser light, when the photon energy is lower than their electron affinity; conversely, the unwanted anions get detached when the photon energy is higher than the electron affinity. This situation is given for ^{36}Cl vs. ^{36}S with 532 nm photons. ILIAMS arrives at such perfection that ^{36}S is suppressed by more than 12 orders of magnitude and particle identification is not necessary any more. However, dissociation of molecules in the accelerator is still important. A similarly advantageous situation occurs for the anions of AlO vs. MgO , paving the way to measuring ^{26}Al , an important radioisotope for geological dating, with high efficiency and with unprecedented sensitivity in the 10^{-16} range.

Further exploration of this new technique aims at measuring fission fragments to trace environmental transport processes, e.g. ^{99}Tc and ^{135}Cs .

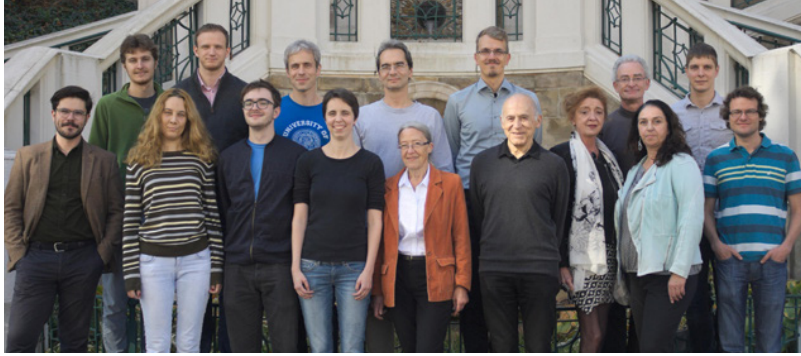
Prizes and awards

Dr. Jenny Feige, now at Berlin, received 2015 the “*Promotionspreis der Fachgruppe Nuklearchemie der Gesellschaft deutscher Chemiker e.V.*” for her doctoral thesis “*Supernova-produced Radionuclides in Deep-Sea Sediments measured with AMS*”. For “*an exceptionally vivid paper about her thesis*”, Jenny received the “*Klaus Tschira Preis für verständliche Wissenschaft*”.

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Mathematical Physics



The Mathematical Physics group studies mathematical and theoretical questions in string theory, gravitational theories and quantum field theory. A main driving force is the question how gravity, as described by Einstein's general theory of relativity, can be reconciled with quantum physics. In particular, as general relativity is a theory of curved space-time geometry, it is expected that any quantum theory of gravity will lead to generalisations of classical geometric concepts. By studying generalised gravitational theories, string theory compactifications, and field theories on non-commutative space-times the group explores different approaches towards a better understanding of the fundamental question: What are space and time?

Research Highlights

A prominent candidate for a quantum theory of gravity is *string theory*. It provides a natural realisation of the graviton as an elementary excitation of a closed string. On the other hand it needs to be supplemented by extra degrees of freedom in addition to the four space-time dimensions that we experience. These usually go under the name of extra dimensions or string compactifications, but they do not need to have a geometric description. The understanding of the structure of such compactifications is vital: phenomenologically - to connect string theory with particle physics - as well as conceptually. Intimately connected to that are a lot of interesting mathematical structures that can lead to a fruitful interplay of physics and mathematics. In this context, Stefan Fredenhagen has explored the description of fusion of defect lines in two-dimensional supersymmetric Landau-Ginzburg models which describe string theory compactifications. Using similar two-dimensional theories, Johanna Knapp (in collaboration with A. Caldeara, Univ. of Wisconsin, and E. Sharpe, Virginia Tech) has found novel realisations of certain Calabi-Yau compactifications [1].

An exciting generalisation of gravity is provided by *higher-spin gauge theories*. They can be understood as an extension of the spin-2 gauge theory that describes gravity (the spin-2 excitation being the graviton) by similar gauge fields of higher spins. There are many indications that higher-spin gauge theories are related to string theory in the limit of tensionless strings. Higher-spin theories lead to mind provoking generalisations of geometry, in which notions of length and time and even causal structures have to be rethought completely. The group has focussed on higher-spin gauge theories in three space-time dimensions which have simpler realisations than their higher-dimensional versions. Jan Rosseel (in collaboration with E. Bergshoeff, Groningen, D. Grumiller, and S. Prohazka, TU Vienna) has explored non-relativistic and ultra-relativistic variants of spin-3 gauge theories in [2]. In [3], Stefan Fredenhagen (in collaboration with A. Campoleoni, Zu-

rich, and J. Raeymaekers, Prague) has shown how a different gauge choice can be used to obtain an improved understanding of quantum aspects of three-dimensional higher-spin gauge theories.

Another approach to understand quantum aspects of geometry is to study *field theories on non-commutative spaces*. Such non-commutative or fuzzy spaces also arise naturally in matrix theories which should be thought of providing a non-perturbative formulation of string theory. Such spaces and the resulting physics are being studied by Harold Steinacker and Marcus Sperling. Recent results [4,5] include the discovery that certain covariant quantum spaces arise as solutions in this model, and provide the ingredients for a higher-spin gauge theory, including the spin-2 sector required for gravity. A particular highlight are cosmological FRW-spacetimes with a regularized Big Bang [6]. A related line of research of Harold Steinacker and Marcus Sperling focuses on fuzzy extra dimensions arising within Yang-Mills gauge theories with large rank. Non-commutative geometries also feature in the work of Harald Grosse, who has investigated quantum field theories on non-commutative Moyal spaces. In this context he has shown (in collaboration with R. Wulkenhaar, Münster) that a scalar field theory on a four-dimensional Euclidean space with a quartic interaction has a solution [7]. In a theory with cubic interaction he could also prove (in collaboration with A. Sato, Tokyo, and R. Wulkenhaar, Münster) that the correlation functions satisfy Osterwalder-Schrader positivity and can thus be analytically continued to Minkowski space-time.

Gravity can be generalised in a number of ways. A supersymmetric version, supergravity, can be obtained as a low energy limit of string theory. In three dimensions also massive versions of gravity have been considered. Such theories are not only interesting tools to understand gravity, but also have relations to condensed matter physics. For this application one has to study the *non-relativistic limit* of such theories, which has been a focus in the research of Jan Rosseel. In [8] (in collaboration with E. Bergshoeff, Groningen, and P. Townsend, Cambridge) he has shown that the Schrödinger equation obeyed by the Girvin-Macdonald-Platzman mode that appears in the Fractional Quantum Hall effect can be derived from the non-relativistic limit of the parity-preserving Fierz-Pauli theory for a real spin-2 field in three dimensions.

In addition to studying condensed matter systems as non-relativistic limits of field theories,

collective quantum phenomena have also been studied directly in *many body quantum theory*. Heide Narnhofer has studied quantum fluctuations in mesoscopic systems in [9] (in collaboration with F. Benatti, F. Carollo and R. Floreanini, Trieste) discovering new features of long range quantum correlations. Jakob Yngvason has investigated the relation of superfluidity and Bose-Einstein condensation. In [10] (in collaboration with M. Könenberg, T. Moser, and R. Seiringer) he has shown in a one-dimensional model of interacting bosons that depending on the chosen parameters one can have complete Bose-Einstein condensation with arbitrary small or with complete superfluidity. In an investigation of the incompressibility of Quantum Hall fluids he has proved (in collaboration with E. H. Lieb, and N. Rougerie) upper bounds on the one-particle density of many-body states in the Laughlin phase.

Selected Publications

- [1] A. Caldeararu, J. Knapp and E. Sharpe, “GLSM realizations of maps and intersections of Grassmannians and Pfaffians,” arXiv:1711.00047 [hep-th].
- [2] E. Bergshoeff, D. Grumiller, S. Prohazka and J. Rosseel, “Three-dimensional Spin-3 Theories Based on General Kinematical Algebras,” JHEP **1701** (2017) 114, doi:10.1007/JHEP01(2017)114, [arXiv:1612.02277 [hep-th]].
- [3] A. Campoleoni, S. Fredenhagen and J. Raeymaekers, “Quantizing higher-spin gravity in free-field variables,” arXiv:1712.08078 [hep-th]. (Accepted at Journal of High Energy Physics)
- [4] H.C. Steinacker, “Emergent gravity on covariant quantum spaces in the IKKT model,” JHEP **1612** (2016) 156, doi:10.1007/JHEP12(2016)156, [arXiv:1606.00769 [hep-th]].
- [5] M. Sperling and H.C. Steinacker, “Covariant 4-dimensional fuzzy spheres, matrix models and higher spin,” J. Phys. A **50** (2017) no.37, 375202, doi:10.1088/1751-8121/aa8295, [arXiv:1704.02863 [hep-th]].
- [6] H.C. Steinacker, “Cosmological space-times with resolved Big Bang in Yang-Mills matrix models,” arXiv:1709.10480 [hep-th]. (Accepted at Journal of High Energy Physics)
- [7] H. Grosse and R. Wulkenhaar, “On the fixed point equation of a solvable 4D QFT model,” Vietnam Journal of Mathematics **44**(2016)153-180, [arXiv:1505.05161 [math-ph]].
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News

- After the retirement of Jakob Yngvason (emeritus status since October 2014), the group has been reshaped with the arrival of Stefan Fredenhagen as professor for Mathematical Physics in September 2016. The group has grown significantly since then: Starting from one (non-retired) group member (Harold Steinacker) in August 2016, resulting in seven group members in December 2017 (plus five master students), with three further appointments already decided for 2018.
- Harold Steinacker has been successful with a FWF grant application, within which Marcus Sperling has been hired in October 2016 as a postdoc for two years.
- Jan Rosseel, expert on supergravity and Newton-Cartan geometry, has joined the group on a long term postdoc position in October 2016.
- Olaf Krüger has joined the group on a long term postdoc position in January 2017 after finishing his Ph.D. on gauged supergravity theories.
- In October 2017, Johanna Knapp, expert on mathematical string theory, has joined the group on a long term postdoc position.
- Pascal Anastasopoulos has been successful with a FWF grant application for a project that he is pursuing as PI in the group since December 2017. His research focuses on string theory and its phenomenological implications, in particular in view of experimental data expected from LHC at CERN and recent astro-particle experiments.
- The group is actively involved in activities at the Erwin Schrödinger International Institute for Mathematics and Physics, for which Stefan Fredenhagen is member of the Scientific Governing Board. Harald Grosse has organised a program on ‘Higher structures in string theory and QFT’ (6 Nov - 18 Dec 2015 with D. Stevenson and R. Szabo), and a workshop on ‘The interrelations between mathematical physics, number theory and non commutative geometry’ (2-13 Mar 2015 with R. Nest, W. Van Suijekom, and St. Weinzierl) including lectures by A. Connes. Stefan Fredenhagen, Harald Grosse, Heide Narnhofer and Jakob Yngvason (together with further colleagues from other groups) organised a memorial symposium on the occasion of the 90th birthday of Walter Thirring on 29 Apr 2017. Several future workshops and programs planned by Stefan Fredenhagen, Harald Grosse, and Harold Steinacker have already been approved.
- H. Steinacker serves as core group member of the COST program MP1405 Quantum structure of spacetime (QSPACE). He was organizer for the COST training school ‘Quantum Structure of Spacetime and Gravity’, Belgrade, Serbia, 21-28 August 2016, for the workshop on Noncommutative Field Theory and Gravity in Corfu, a meeting ‘Quantum gravity, noncommutative and quantum geometries’ within the 37th Max Born Symposium in Wroclaw, and a 2-day workshop ‘Noncommutative Geometry and Gravity’ at the ESI Vienna, Austria, 6-7 June 2017.
- We run a regular research seminar with international speakers and host visits of guest researchers including Anton Alekseev (Geneva), Yuhma Asano (Dublin), John Barrett (Nottingham), Eric Bergshoeff (Groningen), Rutger Boels (Hamburg), Maja Buric (Belgrade), Andrea Campoleoni (Brussels), Thanasis Chatzistravakidis (Zagreb), Stefano Cremonesi (Durham), Khrystyna Gnatenko (Lviv), Yang-Hui He (London), Jnanadeva Maharana (Bhubaneswar), Sanjaye Ramgoolam (London), Tristan McLoughlin (Dublin), Joris Raeymaekers (Prague), Andjelo Samsarov (Zagreb), Juraj Tekel (Bratislava), Miguel Tierz (Lisbon), Cedric Troessaert (Potsdam), Raimar Wulkenhaar (Münster).
- The group has a strong dedication for good teaching, which has been appreciated by the students in an evaluation that put three group members among the four lecturers who were ranked highest, with Olaf Krüger winning the teaching award 2017/18.

Particle Physics

Fields of Research

The research work of the theoretical particle physics group in the years 2015 to 2017 focused on jet physics involving heavy quark flavors and the top quark relevant for the Large Hadron Collider and the future Linear Colliders, dark matter, effective field theories, physics of the standard model at low energies, phenomenology of the Higgs boson in super-symmetric theories, neutrino physics, extensions of the standard model, as well as tests of the foundations of quantum mechanics in particle physics and studies of dynamical systems.

News and Events

University assistant Dr. Vicent Mateu left our working group in October 2015 to take up a Ramón y Cajal research professorship at the University of Madrid from where he moved to the University of Salamanca in December 2016. University assistant Dr. Massimiliano Procura started a two-year leave of absence to CERN for a Marie Curie fellowship in September 2015 and rejoined the group in October 2017. In October 2015 until September 2017, Dr. Yu-Ming Wang, coming from the Technical University Munich, joined our group as a University assistant. Dr. Simon Plätzer, coming from the Universities of Durham and Manchester, was visiting guest professor in the faculty in the summer term 2017 and then joined the group as a University assistant in October 2017. Prof. Jürgen Reuter, coming from DESY Hamburg, was visiting guest professor in the faculty in the summer term 2017. Dr. Aditya Pathak, coming from the Massachusetts Institute of Technology, joined the group as research postdoc in September 2017. Benjamin Rogers joined the group as a postdoc from May until October 2015. Elke Aeikens, Maximilian Löschner, Christopher Lepenik and Daniel Lechner started their PhD studies under the supervision of Walter Grimus and André Hoang within the Doktoratskolleg “Particles and Interactions” (DKPI). Bahman Dehnadi graduated summa cum laude in October 2015. In December 2017 the DKPI was successfully reapproved for its second

funding phase covering from March 2018 until February 2022. The FWF projects “One-loop fermion mass corrections and flavour symmetries” (P 28085-N27, from September 2015) by Walter Grimus and “Heavy quark masses from jets using effective field theory” (P 28535-N27 from July 2017) by André Hoang have been approved. Since November 2016 André Hoang and Simon Plätzer are members of the COST Action Nr. 16201 “Unravelling new physics at the LHC through the precision frontier”, and Simon Plätzer has initiated a partnership agreement with the MCnet3 network.

From July 22-29 members of the group organized the International Conference on High-Energy Physics of the European Physical Society, which was, with more than 750 participants, the major convention event of the particle physics community in 2015 and also had an extended outreach program. The event was hosted in the main building of the University of Vienna and was coorganized with members of the High Energy Physics Institute (HEPHY), the Stefan Meyer Institute for Subatomic Physics (SMI) and the Vienna University of Technology. From November 27 – 28 in 2015, December 1 – 2 in 2016 and November 30 – December 1 in 2017, the group hosted the 11th, 12th and 13th “Vienna Central European Seminar on Particle Physics and Quantum Field Theory” on the topics “Quantum and Gravity” (at the Faculty of Physics, organized by Walter Grimus, Daniel Grumiller (TUV) and Andreas Ipp (TUV)), “Physics at the LHC – Run 2” (at the Natural History Museum, organized by André Hoang, Massimiliano Procura, Joseph Pradler (HEPHY), Jochen Schieck (HEPHY) and Anton Rebhan (TUV)) and “Indirect Searches for New Physics” (at the SKY Lounge of the University of Vienna, organized by Hartmut Abele (TUV), and Walter Grimus), respectively. Each seminar was attended by more than 90 participants and had strong participation of the group members. The Faculty of Physics and the DKPI were important sponsors of both events.

The annual lecture series of the “Erwin Schrödinger Visiting Professorship” kindly supported by the Kulturabteilung der Stadt Wien,

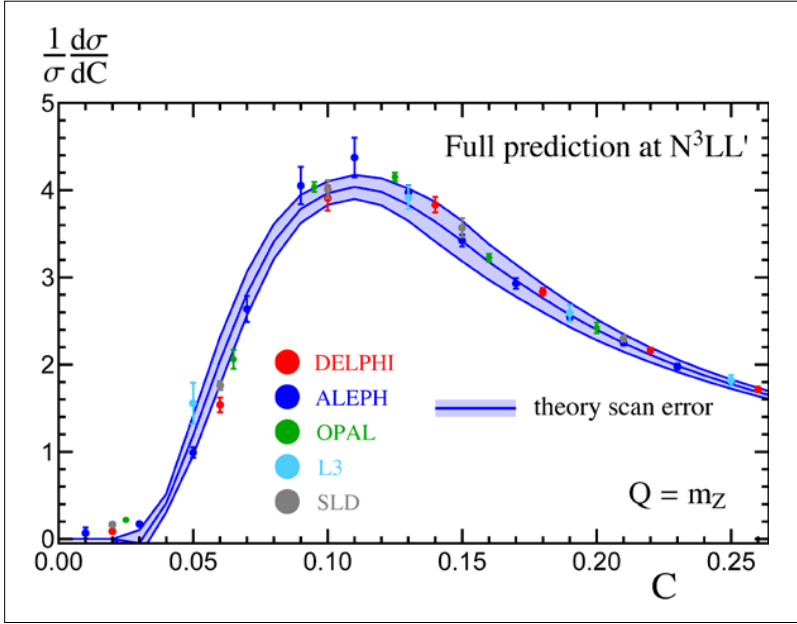


Figure 1

were given by Prof. John F. Donoghue (University of Massachusetts) in 2015 on an effective field theory approach to quantum gravity, by Iain W. Stewart (Massachusetts Institute of Technology) in 2016 on jet physics and by Christopher Sachrajda (University of Southampton) on lattice gauge theory. The lectures took also place in the framework of the DKPI and were attended by members of all participating institutions.

Research Highlights

Currently, neutrino physics seems to be the only window to physics beyond the Standard Model. The discovery of neutrino oscillations, which was rewarded by the Nobel Prize of 2015, has established that neutrinos have mass and the lepton sector possesses a mixing matrix just as the quark sector. The investigation of mechanisms for the generation of neutrino masses and lepton mixing is the research topic of the neutrino physics group. Elke Aeikens and Walter Grimus have studied lepton-flavour violating charged-lepton decays in a neutrino-mass model with soft lepton-flavour violation and demonstrated that the branching ratios of such decays could be close to their respective experimental upper bounds [1]. Predictive neutrino mass and mixing models always have an extended scalar sector and, therefore, a proliferation of Yukawa couplings and vacuum expectation values. Maarten Fox, Walter Grimus and Maximilian Löschner have devised a renormalization scheme for such models which can cope with these complications and allows one to compute radiative corrections to neutrino masses and mixing [2]. Presently, Grimus and Löschner apply

this scheme to the multi-Higgs doublet Standard Model.

The top quark is the heaviest known elementary particle and plays an important role in theoretical considerations concerning the vacuum structure and in physics beyond the Standard Model. The group of André Hoang achieved for the first time a systematic analysis concerning the field theoretic interpretation of top quark masses in the context of Monte-Carlo (MC) event generators, which are currently used in experimental LHC top quark analyses. The work included theoretical calculations using factorization in the context of soft-collinear effective theory at next-to-next-to leading logarithmic (N^2LL) order for boosted top quarks in electron-positron annihilation and involved extensive numerical fits to MC pseudo data [3]. The results were subsequently expanded to proton-proton collisions at the LHC accounting for the effects of soft drop jet grooming [4], which is mandatory to remove underlying event and pileup effects which are hard to describe theoretically. For the top quark mass a formalism was developed which allows to factorize the effects of the lighter bottom and charm quarks in a novel renormalization group formalism. The group also carried out a determination of the strong coupling constant α_s at next-to-next-to-next-to leading logarithmic (N^3LL) order from an analysis of the C-parameter event-shape distributions using available experimental data from electron-positron collisions [5] (see Fig. 1). Furthermore, new measurements of the charm and bottom quark masses were achieved using QCD sum rules based on $O(\alpha_s^3)$ perturbative results with a new method to estimate the theoretical uncertainties in a reliable manner.

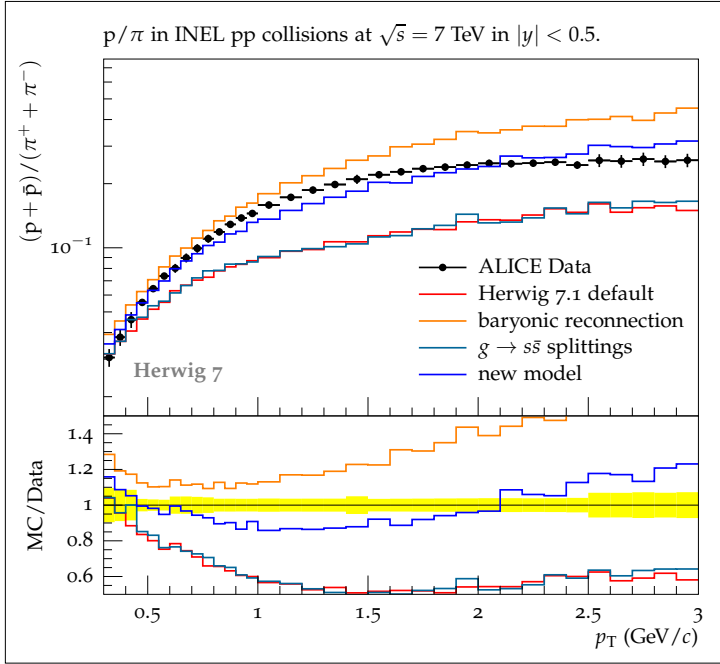


Figure 3

Massimiliano Procura developed a novel theoretical framework based on dispersion relations to achieve the first model-independent, data-driven determination of the hadronic light-by-light contribution to the anomalous magnetic moment of the muon [6]. This work became the Editorial Pick for the cover page of Physical Review Letters (see Fig. 2). This subject was also the subject of his Habilitation which he obtained in October 2017. Procura also introduced a new set of semi-inclusive jet observables which allow us to gain a deeper quantitative insight on distinctive jet substructure characteristics tied to both showering and fragmentation [7]. He also set up the framework to achieve higher logarithmic accuracy and reliable uncertainty estimates for the simultaneous measurements of multiple high-energy QCD observables using Soft-Collinear Effective Theory.

Simon Plätzer has continued to play a major role in advancing the Herwig 7 MC event generator. In particular the consistent combination of NLO QCD corrections to multiple jet production and a significant improvement to the evolution of heavy quarks in the dipole shower are available in release 7.1 [8]. He has also been laying out a new approach to baryon production in the



Figure 2

cluster hadronisation model which improves the description of data substantially [9] (see Fig. 3), and is currently addressing several perturbative and non-perturbative aspects in advancing event generators to precision tools, specifically addressing new evolution algorithms and the foundations of colour reconnection models.

Gerhard Ecker has reviewed the status of chiral perturbation theory for light mesons. In particular, a new global fit of the low energy constants in the strong sector was described. This analysis leads to a prediction of the Cabibbo angle in agreement with the latest lattice determinations. In 2017 he has published a textbook containing an introduction to modern particle physics [10]. Helmut Neufeld has started a new project investigating extensions of the standard model with classical scale invariance. Dmitri Melikhov obtained accurate predictions for the ratios of the decay constants of heavy vector and pseudoscalar mesons using QCD sum rules. It was demonstrated that this ratio is greater than unity for charmed mesons, but is less than unity for beauty mesons, suggesting an unexpected structure of the heavy-quark expansion in QCD.

Alfred Bartl continued his studies of the flavor structure of supersymmetric extensions of the Standard Model. The effects of the mixing between the second and third squark generations on the decays of the Higgs boson into a pair of bottom quarks and a pair of charm quarks we studied taking into account the strong constraints from experimental data on B mesons, limits from supersymmetric particle searches and the mass of the Higgs boson. These effects can lead to deviations of the decay widths from their Standard Model values by up to 30 %.

Helmuth Hüffel proposed a modified Faddeev-Popov path integral density for Yang-Mills theory, where contributions of the Faddeev-Popov ghost fields are replaced by multi-point gauge field interactions. He also studied entanglement of scalar fields on closed compact manifolds. By applying the heat kernel regularization he could show that the field space entanglement entropies of a massless scalar field model and of its Lifshitz dual are agreeing. In the field of dynamical systems, Helmuth Hüffel has introduced a novel type of ergostats and thermostats for molecular dynamics simulations.

All projects were realized with strong local and international collaborations.

Selected Publications

- [1] E.H. Aeikens, W. Grimus, L. Lavoura, Charged lepton decays from soft flavor violation, *Phys. Lett. B* 768 (2017) 365
- [2] W. Grimus, M. Löschner, Revisiting on-shell renormalization conditions in theories with flavour mixing, *Int. J. Mod. Phys. A* 31 (2017) 1630038
- [3] A.H. Hoang, S. Mantry, A. Pathak, I.W. Stewart, Extracting a short distance top mass with light grooming, arXiv: 1708.02586
- [4] M. Butenschoen, B. Dehnadi, A.H. Hoang, V. Mateu, M. Preisser, I.W. Stewart, Top quark mass calibration for Monte-Carlo event generators, *Phys. Rev. Lett.* 117 (2016) 232001
- [5] A.H. Hoang, D.W. Kolodrubetz, V. Mateu, I.W. Stewart, Precise determination of α_s from the C-parameter distribution, *Phys. Rev. D* 91 (2015) 094018
- [6] G. Colangelo, M. Hoferichter, M. Procura, P. Stoffer, Rescattering effects in the hadronic light-by-light contribution to the anomalous magnetic moment of the muon, *Phys. Rev. Lett.* 118 (2017) 232001
- [7] B.T. Elder, J. Thaler, M. Procura, W.J. Waalewijn, K. Zhou, Generalized fragmentation functions for fractal jet observables, *JHEP* 1706 (2017) 085
- [8] J. Bellm, S. Gieseke, S. Plätzer, Merging NLO multi-jet calculations with improved unitarization, arXiv: 1705.06700
- [9] S. Gieseke, P. Kirchgäßer, S. Plätzer, Baryon production from cluster hadronization, *Eur. Phys. J C* 78 (2018) 99
- [10] G. Ecker, Teilchen, Felder, Quanten – Von der Quantenmechanik zum Standard Modell der Teilchenphysik, Springer Spektrum, Juli 2017, ISBN-13: 978-3662545492

Physics of Functional Materials

Research focuses on studying the **physics of functional materials** by experimental, computational and theoretical methods.

Topics cover a broad spectrum, ranging from structural phase transitions and glass transitions, confinement effects of molecular liquids and water in nanoporous systems to the formation and dynamics of domain walls, metal-hydrogen systems, nonlinear light optics and neutron optics, ultra-dense magnetic data storage, detection of tiny magnetic fields and applications for magnetic sensing.

Materials investigated are: multiferroics and magnetic materials, photosensitive materials, soft materials such as nano-composites (polymer-nanoparticle, elastomer-carbon, liquid crystal-polymer), soft and hard magnetic materials.

Techniques employed: nanostructuring of photosensitive materials via nonlinear photonic processes, optical holography, dynamic mechanical analysis, dielectric spectroscopy and 3D printing of magnetic materials. Instruments at large-scale facilities (neutron and synchrotron laboratories) are used for diffuse and inelastic neutron scattering, small-angle scattering, cold neutron optics and interferometry, neutron holography with atomic resolution and 3D X-ray microscopy. Additionally, enhanced simulation tools **for magnetic systems based on finite element and boundary element methods** are developed.

The **retirements** of A. Fuith and H. Kabelka, as well as R. A. Rupp and G. Krexner have left a substantial void. Recalling their contribution of key competences to the group's capacity for both research and teaching over several decades is definitely a matter of concern to us in this context.

Fortunately, the recent **Tenure Track appointment** of Dieter Suess in May 2017, who joined our group with a large number of coworkers, resulted in an eminent boost and gain in research as well as in teaching activities.

R. A. Rupp has been responsible for giving the demanding first year introductory courses in physics since 2011 with an overall number of more than 400 students per year.

Within a long-term project coordinated by our group a series of over 120 lectures with a duration of about 75 minutes each were video-taped by a team led by G. Krexner. The lectures comprise a two-semester Introductory Physics Course and an Introduction to Vector and Tensor Calculus presented earlier by P. Wagner as well as a concise Introduction to Mathematics for Physicists presented by C. Dellago. After considerable editing required due to the use of several cameras the lectures have now become available for the public on a dedicated YouTube channel [1]. The entire project relied on voluntary cooperation of highly motivated students and faculty staff complemented by technical support of the Central Library of Physics and a work station including a video editing system for post production provided by a private sponsor.

The following research projects were granted: FWF-P 28672: "Structure and dynamics of ferroic interfaces" (PI: W. Schranz), ÖAD-WTZ SI 13/2016: "Neutron polarizers based on polymer-nanoparticle composites" (PI: J. Klepp). Christian Doppler Society, "Budget Extension: Advanced Magnetic Sensing and Materials" (PI: D. Suess), ASTC (Seagate, Western Digital, Toshiba), "Reduction of transition curvature in HAMR and outlook for 3D recording" (PI: D. Suess), FFG: "UHF RFID Temperature Sensing" (PI: D. Suess), Frauscher Sensor Technology: "Device Model for Wheel Sensors" (PI: D. Suess)

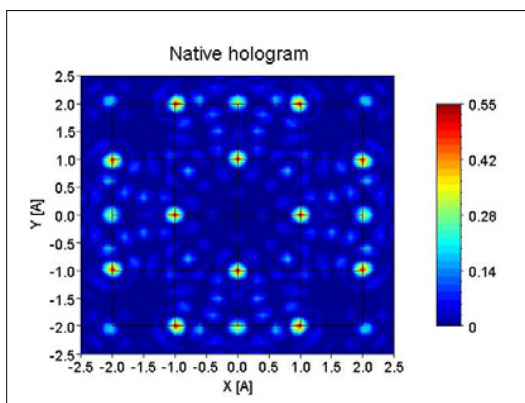


Fig. 1: Neutron-Hologram of a metal-hydrogen system.

More Information: <http://fun.univie.ac.at>

Research Highlights

Neutron holography

G. Krexner

Neutron holography can be an efficient and highly precise tool to investigate the local real-space structure of crystalline materials around specific probe nuclei serving as radiation source or detector (Fig. 1).

Measurements of this type require orientational order and, therefore, restrict the range of study essentially to single crystals. However, if the information searched for is limited to the distances between the probe and the surrounding nuclei instead of their positions, holographic techniques should be applicable to poly-crystalline samples as well. In order to prove this conjecture the expected multi-wavelength holographic signal of a polycrystalline sample was calculated taking into account real instrument parameters [2].

The experimental verification of the predictions can be undertaken at existing pulsed neutron sources. This new method opens the way to expand the field of investigation towards gaining information about the local atomic structure of polycrystalline materials which are of importance also in various applications.

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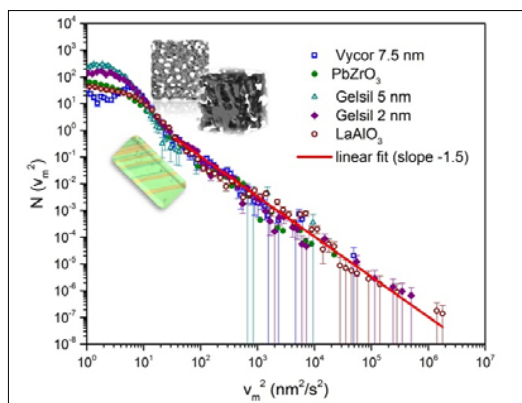


Fig. 2: Gutenberg-Richter law in nanoporous materials and domain wall systems.

From “labquakes” to “earthquakes”

W. Schranz

In this period our research was mainly devoted to the study of so-called “crackling noise” which occurs at the movement of slowly driven interfaces [3],[4] in random environments, e. g. during mechanical failure in nanoporous materials or at dynamic pinning-depinning transitions of ferroelastic domain walls.

The main question is: Can we upscale (Fig. 2) our findings on nanometer sized avalanches to real earthquakes occurring at km size? Or, what do so-called “labquakes” tell us about real earthquakes? In earlier work [J. Baró, Á. Corral, X. Illa, A. Planes, E. K. H. Salje, W. Schranz, D. E. Soto-Parra and E. Vives, *Phys. Rev. Lett.* **110**, 088702, 1-5 (2013)] on acoustic emission (AE) of slowly compressed Vycor we found power-laws in the various distributions recovering the Gutenberg-Richter law, Omori law and Bath’s law, with exponents very similar to those found for real earthquakes, e. g. in California.

In the present period we established a novel complementary (to AE) experimental method for the study of earthquake dynamics. Using a dynamic mechanical analyser (Diamond DMA) we measured strain drops at slowly compressed nanoporous samples. Performing slow compression experiments on Vycor and Gelsil with nanometer pore sizes and in other nanoporous materials like charcoal, sandstone and shist and analysing this big data set using state of the art statistical methods, we obtained valuable insights into the failure dynamics of nanoporous materials and found power law exponents (Fig. 2) that agree very well with those of AE and with theoretical calculations. Very recently, we found power-law behaviour also at pinning-depinning transitions of slowly driven ferroelastic domain walls.

These results demonstrate that the proposed method of measuring strain drops with DMA at slowly varying stress could become a complementary tool for the study of elastic interfaces, avalanches and earthquake dynamics in micron-sized materials. A comprehensive overview is published in a Springer Book on “*Avalanches in functional materials & geophysics*” [5][4].

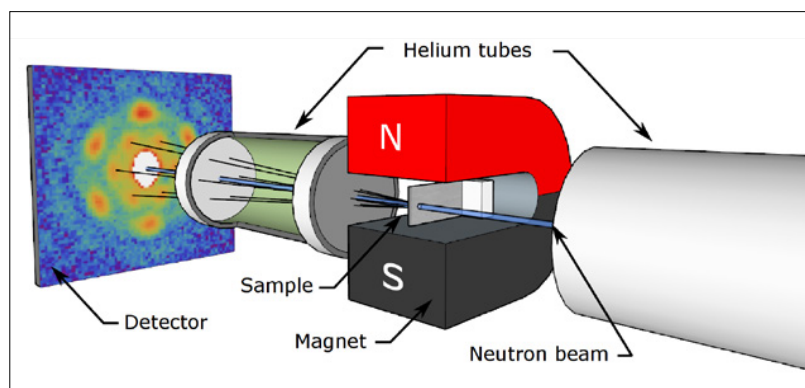


Fig. 3: Sketch of very cold neutron optics setup at the VCN-beamline PF2 (Institut Laue-Langevin).

Optical holography and neutron optics

R. A. Rupp, M. Fally, J. Klepp

Our efforts to combine the holographic technique and the materials aspect for high performance light-sensitive media are focused on multiply doped LiNbO_3 , nanoparticle-polymer composites, liquid crystalline elastomers, and ionic-liquid polymers.

For the classical electrooptic materials we were able to show that optical damage resistance and photorefraction can be simultaneously enhanced, properties that were thought to be contradictory [6]. Preparing high quality one-dimensional photonic crystals from various polymer composites or self assembling colloidal crystals are primarily intended for use as neutron optical components [7].

Optimization of the chemical and physical processes and materials is extremely important whenever applications are envisaged. Progress along this direction over the last decade was extensively reviewed recently [8]. Intriguing diffractive properties of e.g. polarization gratings were discovered and explained: holograms recorded with mutual orthogonal polarization states in strongly dichroitic liquid crystalline elastomers exhibit a profound minimum at the Bragg position rather than a maximum as usually expected [9].

Magnetic Structures for Storage and Sensing

D. Suess, C. Vogler

The focuses of research of our group are fundamental understanding of magnetic effects, functional magnetic structures for sensor and storage applications. This applied research is done in close cooperation with companies worldwide.

One highlight which emerged from the cooperation with Infineon AG within the framework of the Christian Doppler Laboratory is discussed in the Science Outreach 2015 section: “Christian Doppler Laboratory: Advanced Magnetic Sensing and Materials”.

Research highlights in the field of magnetic storage were funded by the ASTC (consortium consisting of Western Digital, Seagate, Toshiba and others) and a WWTF project.

Here we investigated a new magnetic recording scheme that utilizes highly focused laser beams in order to locally heat up recording media above the Curie temperature. The laser beam is focused using a near field transducer and plasmonic resonances well below the diffraction limit (full width at half maximum as small as 20-30 nm). In order to define the orientation of the written bit during cooling a magnetic field is applied in addition to the laser light.

Usually, due to the shape of the laser spot that can be approximated as a Gaussian beam, the written magnetic bit has a circular shape. However, the magnetic reader element that is based on the effect of tunneling magnetoresistance has a rectangular shape. Hence, most preferably the written bit should also have a rectangular shape in order to prevent or limit interactions between adjacent bits during reading.

Within the work discussed in [10] the interplay between the heat gradient, due to the laser spot, and the field gradient of the recording head is utilized to reduce the circular curvature of the written bit pattern. In Fig. 4 one bit (red area) of a current recording design is shown (right). This proposed design requires only feasible changes in the design of the write head and the near field transducer. The theoretical work [10] shows a reduction of the transition curvature of up to 40 % (Fig. 4, left). Estimates on the increase in storage density due to this design are the scope of current research in our group.

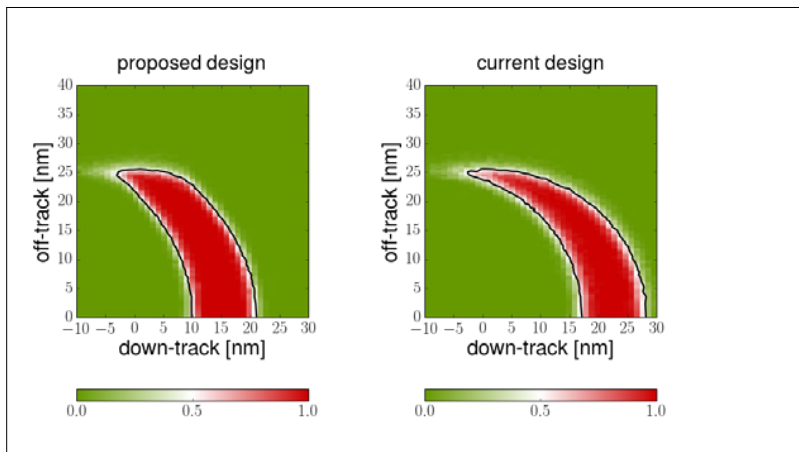


Fig. 4: Written bit (red) with heat assisted recording (HAMR). (right) the conventional design shows significant bit curvature. (left) the proposed design significantly decreases the curvature and allows for higher data densities due to a reduction in read noise.

- [1] <https://www.youtube.com/channel/UCt6PF5PmX-FwzHCTdlc8X2fw>
- [2] A. Szakál, M. Markó, **G. Krexner**, L. Cser, EPL 111, 26002 (2015). DOI: 10.1209/0295-5075/111/26002
- [3] **S. Puchberger**, **V. Soprunyuk**, A. Majchrowski, K. Roleder and **W. Schranz**, Phys. Rev. B 94, 214101 (2016). DOI: 10.1103/PhysRevB.94.214101
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- [9] M Prijatelj, M A Ellabban, **M Fally**, V Domenici, M Čopič, I Drevenšek-Olenik, Opt. Mater. Express 6, 961 (2016). DOI: 10.1364/OME.6.000961
- [10] **C. Vogler**, **C. Abert**, **F. Bruckner**, **D. Suess**, Applied Physics Letters, 110, 182406 (2017). DOI: 10.1063/1.4981805

Physics of Nanostructured Materials

During 2015–2017, PNM group members have celebrated several substantial scientific achievements, promotions, prizes and awards. In February 2017, Jani Kotakoski was awarded tenure and the title “Associate Professor” by the Rector. His research has put the group at the international forefront in the field of irradiation effects in 2D materials and low-dimensional carbon nanostructures. In 2017, Toma Susi was awarded the prestigious ERC Starting Grant to pursue experiments on atomically precise manipulations using transmission electron microscopy, and Michael Zehetbauer was awarded the renowned Tammann Prize of the Deutsche Gesellschaft für Materialkunde for his substantial scientific achievements in the field of severe plastic deformation and nanostructured materials. Further, in 2015 Michael Zehetbauer received the Award from the Materials Science Faculty of Warsaw University of Technology, Warszawa, Poland, for his successful achievements in the field of SPD processed nanomaterials. Giacomo Argentero received the Fritz Grasenik Award of the Austrian Society for Electron Microscopy for his work revealing the 3D atomic structure of a suspended graphene/hBN van der Waals heterostructure, and Gregor Leuthner was awarded the uni:docs fellowship of the University of Vienna to carry out a PhD study on spatially localized chemistry in the electron microscope under the supervision of Jani Kotakoski. For the presentation of his work on the catalytic reaction of Ni with diamond, Semir Tulić was awarded the Dr. Tasilo Prnka Prize at the Nanocon 2017 conference. Thomas Waitz became a Visiting Professor at the International Research Organization for Advanced Science and Technology of the Kumamoto University, Japan. Finally, the outstanding research of Jannik Meyer has been reflected by his inclusion in the Thompson-Reuters annual list of highly cited researchers in years 2015–2017.

Research Highlights

One way to gain control over the properties of materials is the controlled introduction of imperfections, such as foreign lattice atoms or, in the case of 2D materials, out-of-plane corrugations.

In the awarded work of Giacomo Argentero et al., a novel detection scheme allowed us to demonstrate that a free-standing van der Waals heterostructure consisting of graphene and hexagonal boron nitride with slight misorientation can exhibit an intrinsic buckled atomic structure (Fig. 1). This rippling arises from fluctuations in the van der Waals interaction between two materials, and it also affects the strain within each layer. The work provides important insights into effect of the van der Waals interaction on the individual materials in the new research field of layered 2D heterostructures. (G. Argentero, A. Mittelberger, M. R. A. Monazam, Y. Cao, T. J. Pennycook, C. Mangler, C. Kramberger-Kaplan, J. Kotakoski, A. K. Geim, J. C. Meyer: Unraveling the 3D atomic structure of a suspended graphene/hBN van der Waals heterostructure, *Nano Letters* 17, 1409 (2017) <http://dx.doi.org/10.1021/acs.nanolett.6b04360>)

In work related to the ERC grant of Toma Susi, published in the journal *Ultramicroscopy*, we recently demonstrated for the first time a controlled relocation of an impurity atom (silicon) in the graphene lattice over multiple steps (Fig. 2). Between the overview images shown, the atomically small electron beam was placed on the position marked by the white dot for 10 s to initiate a dynamic process leading to the movement of the Si atom. This approach provides nanotechnology a new method for atom-by-atom construction of structures, as also explained in our recent perspective article in *2D Materials*. (T. Susi, J. C. Meyer, J. Kotakoski: Manipulating low-dimensional materials down to the level of single atoms with electron irradiation, *Ultramicroscopy* 180, 163 (2017) <https://doi.org/10.1016/j.ultramic.2017.03.005>; T. Susi, D. Kepaptsoglou, Y.-C. Lin, Q. Ramasse, J. C. Meyer, K. Suenaga & J. Kotakoski: Towards atomically precise manipulation of 2D nanostructures in the electron microscope, *2D Mater.* 4, 042004 (2017) <http://dx.doi.org/10.1088/2053-1583/aa878f>)

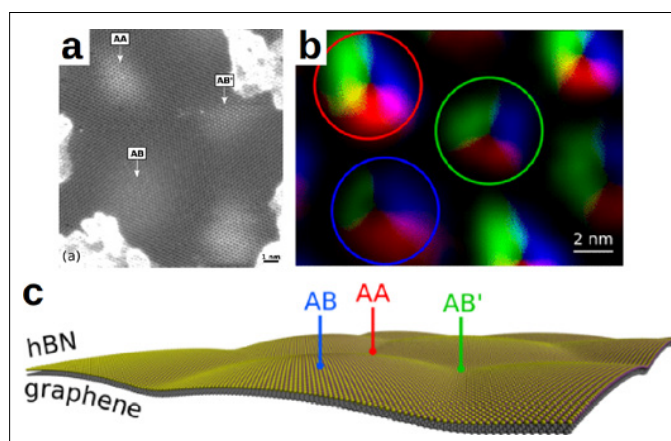


Fig. 1: Medium-angle annular dark field STEM image (a), directional scattering map (b) and structural model (c) of a graphene-hexagonal boron nitride heterostructure (Nano Lett. 2017).

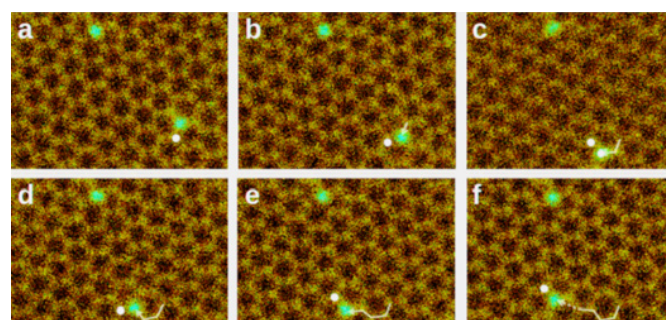


Fig. 2: Controlled displacement of a Si impurity in graphene (Ultramicroscopy 2017).

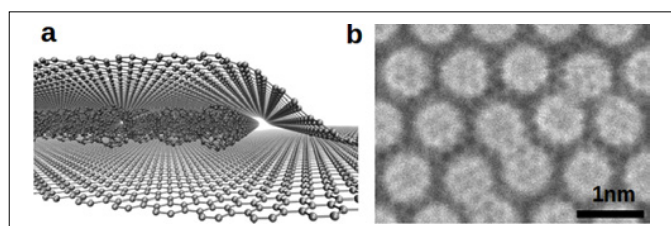


Fig. 3: (a) Illustration and (b) experimental image of C60 fullerenes between two graphene sheets (Science Advances 2017).

Razim Mirzayev, Kimmo Mustonen et al. demonstrated the first direct images of a suspended 0D/2D heterostructure that incorporates C60 molecules between two graphene layers in a buckyball sandwich structure. Clean and ordered C60 islands with thicknesses down to one molecule could be observed. The fullerene monolayers inside the sandwich exhibited a lattice spacing of 9.6 \AA , $\sim 5\%$ smaller than the bulk spacing (Fig. 3). The diffusion dynamics of entire fullerenes could be directly followed, as well as the fusion of fullerenes under high electron doses. The sandwich structure serves as a 2D nanoscale reaction chamber, allowing the analysis of the structure of the molecules and their dynamics at atomic resolution. (R. Mirzayev, K. Mustonen, M. R. A. Monazam, A. Mittelberger, T. J. Pennycook, C. Mangler, T. Susi, J. Kotakoski, J. C. Meyer: Buckyball sandwiches, *Science Advances* 3, e1700176 (2017) <http://dx.doi.org/10.1126/sciadv.1700176>)

In the field of metallic glasses, Christian Rentenberger and his co-workers published a novel technique to measure the atomic-level elastic strain and to probe structural rearrangements during deformation by local electron diffraction. This method was used to monitor anelastic properties of TiAl thin films. (C. Ebner, R. Sarkar, J. Rajagopalan, C. Rentenberger, *Ultramicroscopy* 165, 51-58 (2016); R. Sarkar, C. Ebner, E. Izadi, C. Rentenberger, J. Rajagopalan, *Mat. Res. Lett.* 5, 135-143 (2017))

In collaboration with international groups medium range-ordered clusters of CuZrAlAg bulk metallic glasses were studied by fluctuation electron microscopy. It could be demonstrated that the structural motifs of the clusters and their dominance in the amorphous alloy are sensitive on the composition and affect the glass-forming ability of the material. (C. Gammer, B. Escher, C. Ebner, A. M. Minor, H. P. Karnthaler, J. Eckert, S. Pauly, C. Rentenberger, *Sci. Rep.* 7, 44903 (2017))

Within the framework of the EU Training Network BIOTINET, a highlight paper showed that the high anisotropy of Ti-Nb alloys yields some of the largest linear thermal expansion coefficients ever reported, and allows for optimum mechanical and functional properties using their complex interplay of diffusive and displacive phase transformations (M. Boenisch, A. Panigrahi, M. Stoica, M. Calin, E. Ahrens, M. Zehetbauer, W. Skrotzki, J. Eckert, *Nature Comm.* 8, 1429 (2017)). Another important study found that the annealing of deformation induced dislocations in semicrystalline propylene observed by in-situ synchrotron X-ray diffraction occurs via back-stress release at the glass transition point and via recrystallization of mosaic crystallites at higher temperatures (F. Spieckermann, G. Polt, H. Wilhelm, M. Kerber, E. Schafner, V. Soprunyuk, M. Reinecker, S. Bernstorff, M. Zehetbauer, *Macromolecules* 50, 6362-6368 (2017)).

Invited Talks

In 2015–2017, members of the group actively disseminated research results in conferences and workshops, including several keynote and invited presentations, for example, in the 2017 conference Microscopy and Microanalysis (M&M), St. Louis, USA (Jannik Meyer and Christian Rentenberger), Nature conference “The future of electron microscopy”, Zhejiang, China (Jannik Meyer), Materials Research Society Fall meeting 2017, Boston, USA (Jani Kotakoski), ICAMD2017, Jeju, Republic of Korea (Jani Kotakoski), Selecta Summer School (*Horizon 2020* Programme), Ionannina, Greece (Thomas Waitz), 3a Escola de Química Computacional, Ribeirão Preto, SP, Brazil (Toma Susi), the Int. Nanomaterials Workshop 2015, Nanjing University, China (2015), and the 2017 Sustainable Industrial Processing Summit & Exhibition (SIPS 2017), Cancun, Mexico (both Michael Zehetbauer).

Research Infrastructure

In 2017 major reconstruction works were undertaken at the PNM laboratory located at Sternwarte (Astronomical Observatory of the University of Vienna) to provide suitable conditions for a new Thermo Fisher/FEI aberration-corrected Titan transmission electron microscope. Equipped with a Cs corrector for the objective lens and a monochromator, the instrument has strong imaging capabilities in the TEM and STEM modes, while also providing versatile analytical methods (e.g., EELS and EDX). In 2016, Erhard Schafner designed a miniaturized high pressure torsion device suitable for obtaining in situ diffraction data using XRD and synchrotron radiation. This unique device has already been used to study the evolution of phases and defects of various materials (e.g., pure elements, alloys and even ceramics) during severe plastic deformation.

Editorial Activities and Conferences

Since 2015, Thomas Waitz has served as an Associate Editor for the new scientific journal “Shape Memory and Superelasticity” of the Springer publishing company. In 2017, Toma Susi joined the advisory panel of the IOP journal Nanotechnology as well as the Young Academy of Europe, becoming at the same time a member of the board. In 2016, Jannik Meyer, Jani Kotakoski and Toma Susi participated in the organization of the Seventeenth International Conference on the Science and Applications of Nanotubes and Low-Dimensional Materials (NT16) at the University of Vienna. In 2015, Michael Zehetbauer and Florian Spieckermann acted as guest editors of an In-Focus publication of the renowned journal “Polymer International” with a number of highlight papers on polymer science from the 6th International Conference on Polymer Behaviour (ICPB 6), which was previously organized by them at the University of Vienna. In 2016, Michael Zehetbauer held the 27th Int. Colloquium on Fatigue Mechanisms Vienna, at the Faculty of Physics, Univ. Vienna.

Outreach Activities

During the years 2015 to 2017, the PNM group has also been active in outreach activities. For example, Daria Setman was engaged in the program “FiT-Frauen in der Technik” as well as in the so-called “Junior Science Club”. She gave a Physics lecture at a high school in Vienna and was also responsible for the visit of the high school class at the Faculty of Physics, providing another physics lecture as well as a guided lab tour. Daria Setman and the teams around Jannik Meyer and Erhard Schafner participated in the Kinderuni event with workshops, and in the Campus Festival that was part of the University’s 650-year celebrations in 2015. The team of Jannik Meyer also participated in the Lange Nacht der Forschung in 2016. In 2015–2017, Christian Rentenberger was a co-ordinator of the Faculty of Physics of Vienna’s Annual Study and Job Fair “BeSt” and participated in the “Speed-Job-Dating” at the Arbeitsmarktservice St. Pölten.

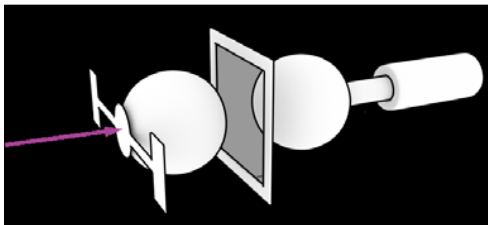
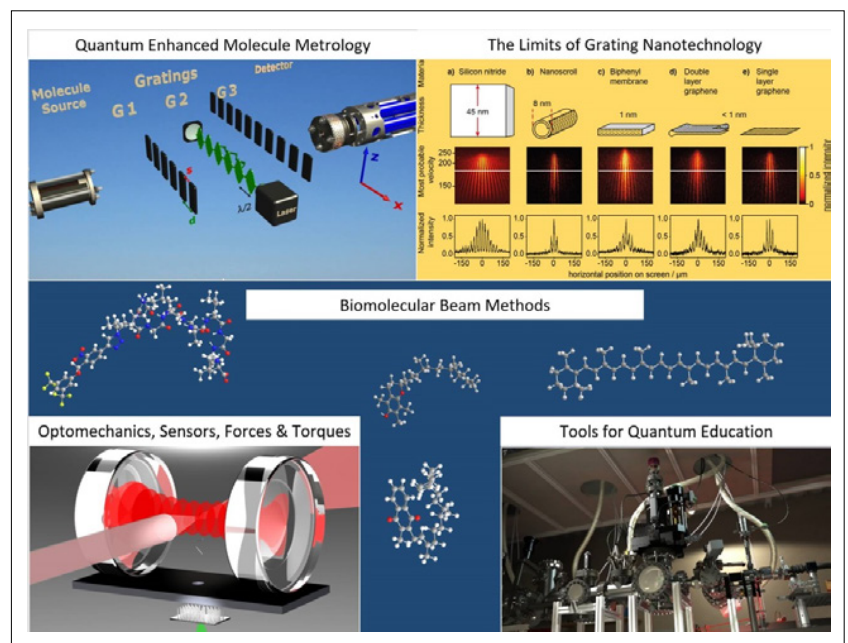
Quantum Optics, Quantum Nanophysics and Quantum Information

The Key Research Area *Quantum Optics, Quantum Nanophysics and Quantum Information* focuses on the foundations and applications of quantum physics by uniting about 100 researchers around Markus Arndt, Markus Aspelmeyer, Časlav Brukner, Ivette Fuentes, Beatrix C. Hiesmayr, Frank Verstraete, Philip Walther and Anton Zeilinger. In 2015-2017 the quantum group published 266 papers, among them 74 in high-impact journals such as *Science*, the *Nature* family and *Physical Review Letters*. They attracted 19 new research grants, such that they had 48 active projects in parallel during the years 2015-2017. Besides, 8 competitive fellowships – for PhDs and postdoctoral researchers – were acquired. In total 24 PhD and 14 Master theses were completed.

Markus Aspelmeyer was awarded a Consolidator Grant of the European Research Council (ERC), Beatrix C. Hiesmayr was elected ERASMUS+ teacher at the King's College London and Philip Walther was elected as a member of the American Physical Society (APS).

Quantum Nanophysics (Arndt group)

The Quantum Nanophysics Group, headed by Markus Arndt, is working on tests of fundamental quantum phenomena and quantum-enhanced precision experiments with biological nanomatter and tailored nanoparticles. We have pushed quantum diffraction to its technological limit using gratings cut in atomically thin graphene [1]. Even in ultrathin masks we found local charges that limit the persistence of quantum coherence for polar biomolecules. In KDTLI interferometry, we have demonstrated that photon absorption in an optical grating for molecules is not necessarily a bad thing but can also serve as a quantum coherent beam splitting mechanism [2]. Biomolecule interference in KDTLI served to explore new



Schematic drawing of the experimental design for a micromechanical measurement of gravitational forces between milligram-scale masses. Shown are (from left to right) the test-mass micromechanical resonator, a membrane to shield electric patch fields, and the millimeter-scale source mass generating time-dependent gravitational fields at the location of the test mass.

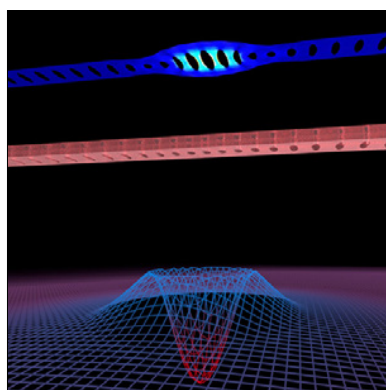
frontiers in quantum assisted metrology with a set of vitamin molecules [3]. We developed methods to launch size-selected nanorods and to see first effects of torsional optomechanics in a high-finesse cavity [4]. With appropriate polarization control, levitated nanorods were shown to then act as a highly accurate mechanical hand of an external clock. Following the drive with better than $1:10^{11}$ in stability. The phase lag of the nanorod turned out to provide a fine tool to measure low gas pressures with unprecedented position resolution and sensitivity.

Selected Publications

- [1] Kuhn, S.; Stickler, B. A.; Kosloff, A.; Patolsky, F.; Hornberger, K.; Arndt, M.; Millen, J., **Optically driven ultra-stable nanomechanical rotor**
Nature Communications 8, 1670 (2017)
- [2] L. Mairhofer, S. Eibenberger, J. P. Cotter, M. Romirer, A. Shayeghi, M. Arndt
Quantum-assisted metrology of neutral vitamins in the gas-phase
Angew. Chem. Int. Ed. 56, 10947 (2017), DOI: 10.1002/anie.201704916
- [3] C. Brand, M. Sclafani, C. Knobloch, Y. Lilach, T. Juffmann, J. Kotakoski, C. Mangler, A. Winter, A. Turchanin, J. Meyer, O. Cheshnovsky, M. Arndt
An atomically thin matter-wave beam splitter
Nature Nanotechnology 10, 845 - 848 (2015) , DOI: 10.1038/nnano.2015.179
Nature Nano: News & Views by P. Treutlein , Highlighted by Physics World
- [4] S. Kuhn, P. Asenbaum, A. Kosloff, M. Sclafani, B. A. Stickler, S. Nimmrichter, K. Hornberger, O. Cheshnovsky, F. Patolsky, and M. Arndt
Cavity-assisted manipulation of freely rotating silicon nanorods in high vacuum
Nano Letters 15, 5604–5608 (2015), DOI: 10.1021/acs.nanolett.5b02302
- [5] J. P. Cotter, S. Eibenberger, L. Mairhofer, X. Cheng, P. Asenbaum, M. Arndt;
K. Walter, S. Nimmrichter, K. Hornberger
Coherence in the presence of absorption and heating in a molecule interferometer
Nature Communications 6, 7336 (2015), DOI: 10.1038/ncomms8336

Quantum Foundations and Quantum Information on the Nano- and Microscale (Aspelmeyer group)

The main research objective in the Aspelmeyer group is to investigate quantum effects of nano- and microscopic systems and their implications for the foundations and applications of quantum physics. We apply and develop quantum optics methods to achieve control over motional states of these systems in the quantum regime. In a series of recent experiments we demonstrated non-classical states of motion comprising single photons and single phonons from a nanomechanical device [1,2]. From an application perspective, such solid-state based photon-phonon interfaces are an interesting platform for quantum information processing architectures. We are also studying the optical control and manipulation of levitated nanoparticles, for which we have now realized optical trapping, manipulation and transport of nanoparticles in an evacuated hollow core photonic crystal (HCPC) fiber [3]. This platform provides added flexibility in the optical micro-manipulation of sub-micron particles in vacuum; at the same time it serves as a new testbed for the study of gasflow in microchannels. The group is particularly interested in the perspectives for studying the interface between quantum physics and gravity using quantum optical control over the motion of increasingly massive solids. Future experiments along this line will require sensitive measurements of small gravitational forces. The group has suggested and analysed an experimental scheme based on micromechanical sensing to observe gravity between milligram-scale source masses, thereby improving the current smallest source mass values by three orders of magnitude and possibly even more [4]. The START group of Nikolai Kiesel studies questions at the interface of thermodynamics, information theory and quantum physics. Recently they have been investigating the performance of an underdamped stochastic heat engine, thereby analytically finding the optimal protocol that maximizes the efficiency at fixed power [5].



Artist impression of a non-classical single-phonon state generated via quantum optical interactions in a nanomechanical system. Shown is, from top to bottom, the displacement field, the nano-optomechanical device and the (negative) Wigner function representing the quantum state.

Selected Publications

- [1] **Hanbury Brown and Twiss interferometry of single phonons from an optomechanical resonator**, S. Hong, R. Riedinger et al., Science 358, 203-206 (2017)
- [2] **Nonclassical correlations between single photons and phonons from a mechanical oscillator**, R. Riedinger, S. Hong et al., Nature 530, 313-316 (2016)
- [3] **Optical trapping and control of nanoparticles inside evacuated hollow core photonic crystal fibers**, D. Grass et al., Appl. Phys. Lett. 108, 221103 (2016)
- [4] **A micromechanical proof-of-principle experiment for measuring the gravitational force of milligram masses**, J. Schmöle et al., Class. Quantum Grav. 33, 125031 (2016)
- [5] **Underdamped Stochastic Heat Engine at Maximum Efficiency**, A. Dechant et al., Euro. Phys. Lett. 119, 50003 (2017)

Quantum Foundations and Quantum Information Theory (Brukner group)

The goal of the group around Časlav Brukner is to gain insights into quantum foundations and quantum information by exploiting operational and information-theoretic approaches. The team has recently applied them to the field of causality and gravity. The group considered low-energy quantum mechanics in the presence of gravitational time dilation and showed that the latter leads to decoherence of quantum superpositions [1]. They continued to study “superpositions of causal orders” in quantum mechanics, collaborating in their verification [2,3] and proving that such a superposition allows for an exponential saving in communication, compared to one-way quantum (or classical) communication [4]. In independent research directions, they found a fundamental limitations to the joint measurability of time along neighboring space–time trajectories, arising from the interplay between quantum mechanics and general relativity [5] and they collaborated on the first test of quantum formulation of the Einstein’s equivalence principle [6].

- [1] **Universal decoherence due to gravitational time dilation**, I. Pikovski, M. Zych, F. Costa, C. Brukner, *Nature Physics* 11, 668–672 (2015)
- [2] **Experimental superposition of orders of quantum gates**, L. M. Procopio, A. Moqanaki, M. Araújo, F. Costa, I. A. Calafell, E.G. Dowd, D. R. Hamel, L. A. Rozema, C. Brukner and P. Walther, *Nature Communication* 6, 7913 (2015)
- [3] **Experimental verification of an indefinite causal order**, G. Rubino, L. A. Rozema, A. Feix, M. Araújo, J. M. Zeuner, L. M. Procopio, Č. Brukner, and P. Walther, *Sci. Adv.* 2017,3: e1602589 (2017)
- [4] **Exponential Communication Complexity Advantage from Quantum Superposition of the Direction of Communication**, P. A. Guérin, A. Feix, M. Araújo and Č. Brukner, *Phys. Rev. Lett.* 117, 100502 (2016)
- [5] **Entanglement of quantum clocks through gravity**, E. Castro, F. Giacomini, Č. Brukner, doi: 10.1073/pnas.1616427114, *PNAS* March 7, 2017
- [6] **Quantum test of the equivalence principle for atoms in coherent superposition of internal energy states**, G. Rosi, G. D’Amico, L. Cacciapuoti, F. Sorrentino, M. Prevedelli, M. Zych, Č. Brukner, and G. M. Tino, *Nature Communications* 8,15529 (2017)

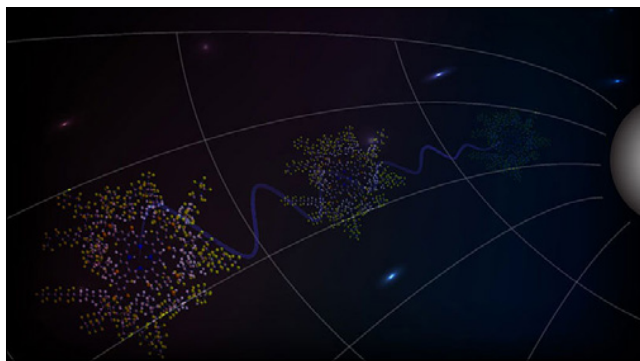


Illustration of a molecule in the presence of gravitational time dilation. The molecule is in a quantum superposition of being in several places at the same time, but time dilation destroys this quantum phenomenon.

Relativistic Quantum Information and Metrology (Fuentes group)

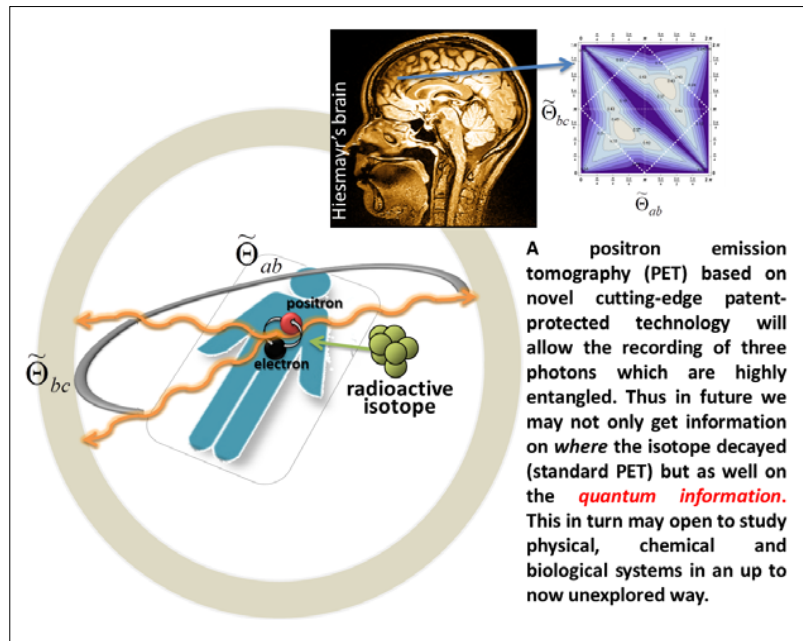
Fuentes’ group worked in the overlap of quantum information, quantum metrology and general relativity. Their research focused on understanding the effects of gravity and motion on quantum properties and their applications in quantum information. Fuentes collaborated with Rupert Ursin (IQOQI) providing theoretical support to the first experiments studying the effects of acceleration on entanglement. These experiments confirmed Fuentes’ theoretical prediction that entanglement is conserved under uniform acceleration. The group also collaborated with C. Wilson at the University of Waterloo who demonstrated experimentally, using superconducting circuits, Fuentes’ scheme for generating quantum gates and multipartite entanglement through relativistic motion. Fuentes’ group searched for ways of exploiting relativistic effects to improve quantum technologies and proposed schemes for using quantum systems to measure gravitational effects including gravitational waves and space-time parameters. They developed methods to apply quantum metrology techniques to relativistic settings using the covariance matrix formalism and quantum field theory in curved space-time. These techniques were used to propose space-based quantum experiments aimed at measuring the Earth’s space-time parameters.

Selected Publications

- [1] Matthias Fink, Ana Rodriguez-Aramendia, Johannes Handsteiner, Abdul Zia-kash, Fabian Steinlechner, Thomas Scheidl, Ivette Fuentes, Jacques Pienaar, Tim C. Ralph, Rupert Ursin, **Experimental test of photonic entanglement in accelerated reference frames**, *Nature Communications* 8, 15304 (2017)
- [2] Roger Penrose and Ivette Fuentes, **Gravitationally induced wavefunction collapse: possible detection by Bose-Einstein condensates**, *Collapse of the Wave Function ('the Work')* edited by Shan Gao ('the Editor') and published by Cambridge University Press (2017)
- [3] Maximilian Lock and Ivette Fuentes, **Dynamical Casimir effect in curved space-time**, *New J. Phys.* 19, 073005, (2017)
- [4] Richard Howl, Lucia Hackermüller, David Edward Bruschi and Ivette Fuentes, **Gravity in the Lab**. Invited review by M. Plenio for *Advances in Physics: X*, 1383184 (2017)
- [5] Jan Kohlrus, David Edward Bruschi, Jorma Louko and Ivette Fuentes, **Quantum communications and quantum metrology in the spacetime of a rotating planet**, *EPJ Quantum Technology* 4:7 (2017)
- [6] N. Liu, J. Goold, I. Fuentes, V. Vedral, K. Modi & D. E. Bruschi, **Quantum thermodynamics for a model of an expanding universe**, *Class. Quantum Grav.* 33:035003 (2016)

Quantum Phenomena at High and Low Energies (Hiesmayr group)

Hiesmayr's group focuses on studying the entanglement and other quantum effects in systems at low and high energies. This covers a broad portfolio of different physical systems such as photons at low/high energies, neutrinos, neutral mesons, condensed matter systems and recently also including operated cancerous/healthy tissues from patients.



In July 2016 a prototype positron-emission tomograph (PET) started operation based on novel cutting-edge patent-protected technology, see e. g. [1]. It will enable recording the frequent decays into three photons during a routine PET-scan that standard PETs have so far never recorded. As shown in [2] the entanglement of the three-photon is genuinely multipartite entangled, a very strong type of entanglement. Surprisingly, this is also the case for the highly mixed case expected for human tissues. Furthermore, experimentally feasible observables to detect different types of genuine multipartite entanglement were developed. Together with another pilot study showing that the lifetimes of ortho-positronium and para-positronium is greater for cancerous tissues than healthy tissues of the same patient, we have a new promising tool at hand that not only the classical but as well the quantum information can be read out during a PET-scan.

For photons at low energy we developed criteria to detect genuine multipartite entanglement efficiently. This allowed the first experimental proof of entanglement of four orbital-angular-momentum entangled photons [3], a joint work with researchers at the Leiden University published in Phys. Rev. Lett. and highlighted by the editor and various other webpages.

Another experimental highlight was based on our theoretical magic simplex studies of the geometry of Greenberger-Horne-Zeilinger (GHZ) states by generating a complete basis with two physical photons entangled in the polarization degrees of freedom and the orbital-angular-momentum degrees of freedom, a joint work with researchers at the University of Rome [4]. We have experimentally proven that there are "twins" in a complete basis set, showing different entanglement features than any other mixture.

Collapse models present one way out of the so called measurement problem, a dedicated experiment based on X-rays, high energetic photons, presents the current world-best upper limit [5] on such models.

Our investigations of collapse models for neutral mesons reveal a new path to explain the decay constants.

For particular condensed matter systems (Ising interaction, nematic & topological phases) the interplay between frustration and entanglement was unveiled by new dedicated measures.

The contextuality, one main ingredient for quantum theory, was studied for decaying systems and accepted by Rapid Communication [6].

Hiesmayr was invited as a distinguished speaker at the 48 Symposium on Mathematical Physics in Torun (Poland) celebrating 40 years "G-K-L-S master equation" due to her contributions to the regime of high energy physics. She runs a Visitor ÖAD programme, Austria-India, on studies of quantum information theoretic tasks in neutrino-oscillations.

Selected Publications

- [1] "Calculation of time resolution of the J-PET tomograph using the Kernel Density Estimation"
L. Raczyński, W. Wiślicki, W. Krzemień, P. Kowalski, D. Alfs, T. Bednarski, P. Białas, C. Curceanu, E. Czerwiński, K. Dulski, A. Gajos, B. Głowacz, M. Gorgol, B. Hiesmayr, B. Jasińska, D. Kamińska, G. Korcyl, T. Kozik, N. Krawczyk, E. Kubicz, M. Mohammed, M. Pawlik-Niedźwiecka, S. Niedźwiecki, M. Pałka, Z. Rudy, O. Rundel, N.G. Sharma, M. Silarski, J. Smyrski, A. Strzelecki, A. Wieczorek, B. Zgardzińska, M. Zieliński and P. Moskal
Phys. Med. Biol. 62, 5076 (2017)
- [2] "Genuine Multipartite Entanglement in the 3-Photon Decay of Positronium"
B.C. Hiesmayr and P. Moskal
Scientific Reports 7: 15349 (2017)
- [3] "Four-photon orbital angular momentum entanglement"
B. C. Hiesmayr, M. J. A. de Dood and W. Löffler
Phys. Rev. Lett. 116, 073601 (2016)
Highlighted by the editor <http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.116.073601> !
And various webpages, e.g. <http://phys.org/news/2016-02-leiden-physicists-entangle-rotating-photons.html>
- [4] "Experimental investigation on the geometry of GHZ states"
G. Carvacho, F. Graffitti, V. D'Ambrosio, B. C. Hiesmayr and F. Sciarrino
Scientific Reports 7:13265 (2017)
- [5] "CSL collapse model mapped with the spontaneous radiation"
K. Piscicchia, A. Bassi, C. Curceanu, R. Del Grande, S. Donadi, B. C. Hiesmayr, A. Pichler
Quantum Information and Foundations, Entropy 19 (7), 319 (2017)
- [6] "Contextuality and Nonlocality in Decaying Multipartite Systems"
Beatrix C. Hiesmayr and Jan-Åke Larsson
Rapid Communication: Phys. Rev. A 93, 020106 (2016)

Many-Body Quantum Theory (Verstraete group)

Frank Verstraete's group focuses on studying the entanglement structure of quantum many body systems, with applications in computational physics, statistical physics, condensed matter physics, quantum field theory and quantum chemistry.

In [1], we devised theoretical tools for quantifying entanglement in gauge theories, thereby solving a long-standing open problem. [2] discusses QED in 1+1 dimensions (the Schwinger model) from the entanglement point of view, and we simulate phenomena such as confinement and string breaking to an unprecedented precision.

We have formulated real-space renormalization group flows in terms of tensor networks, thereby uncovering the limitations of the usual block spin methods and resolving them using entanglement [3]. The tensor network point of view also opens up the possibility of connecting different perturbative expansions through quantum phase transitions, opening up the possibility of studying anyon condensation, confinement and order parameters for topological systems [4].

Selected Publications

- [1] **Entanglement of Distillation for Lattice Gauge Theories**
Karel Van Acoleyen, Nick Bultinck, Jutho Haegeman, Michael Marien, Volkher B. Scholz, and Frank Verstraete
Phys. Rev. Lett. 117, 131602 (2016)
- [2] **Confinement and String Breaking for QED2 in the Hamiltonian Picture**
Boye Buyens, Jutho Haegeman, Henri Verschelde, Frank Verstraete, and Karel Van Acoleyen
Phys. Rev. X 6, 041040 (2016)
- [3] **Renormalization Group Flows of Hamiltonians Using Tensor Networks**
M. Bal, M. Mariën, J. Haegeman, and F. Verstraete
Phys. Rev. Lett. 118, 250602 (2017)
- [4] **Bridging Perturbative Expansions with Tensor Networks**
Laurens Vanderstraeten, Michaël Mariën, Jutho Haegeman, Norbert Schuch, Julien Vidal, and Frank Verstraete
Phys. Rev. Lett. 119, 070401 (2017)

Quantum Information Sciences and Quantum Computation (Walther group)

The Quantum Information Science and Quantum Computation group, headed by Philip Walther, aims to develop new technologies and to exploit those for photonic quantum computation and quantum simulation experiments. In 2015 we demonstrated a new quantum computational architecture that allows for additional computational speed-ups when superimposing also the order of quantum gates [1]. This concept of superimposed temporal orders was further verified by a complex interferometer [2]. The usage of metamaterials has allowed us to obtain experimental benchmark values for hyper-complex extension of quantum mechanics that rely on quaternions instead of complex numbers [3]. Regarding the promising architectures for resource-efficient photonic quantum computers that exploit multi-photon interference in optical networks, we have investigated the general case of multi-photon quantum interference using waveguide structures [4]. For secure quantum computing, where the client's data and software remain private, we have demonstrated a feasible protocol for blind quantum computing where in contrast to previous protocols the client just needs to measure single photons for controlling the computation.

Selected Publications

- [1] **Experimental Superposition of Orders of Quantum Gates**, L. M. Procopio et al., Nature Communications 6, 7913 (2015)
- [2] **Experimental Verification of an indefinite Causal Order**, G. Rubino, L.A. Rozema, A. Feix, M. Araújo, J.M. Zeuner, L.M. Procopio, C. Brukner, P. Walther, Science Advances 3, e1602589 (2017)
- [3] **Single-photon test of hyper-complex quantum theories using a metamaterial**, L.M. Procopio, L.A. Rozema, Z. Jing Wong, D.R. Hamel, K. O'Brien, X. Zhang, B. Dakic, P. Walther, Nature Communications 8, 15044 (2017)
- [4] **Generalized Multiphoton Quantum Interference**, M. Tillmann et al., Physical Review X 5, 041015 (2015)
- [5] **Demonstration of measurement-only blind quantum computing**, C. Greganti, M.-C. Roehsner, S. Barz, T. Morimae, P. Walther. New Journal of Physics 18, 013020 (2016)

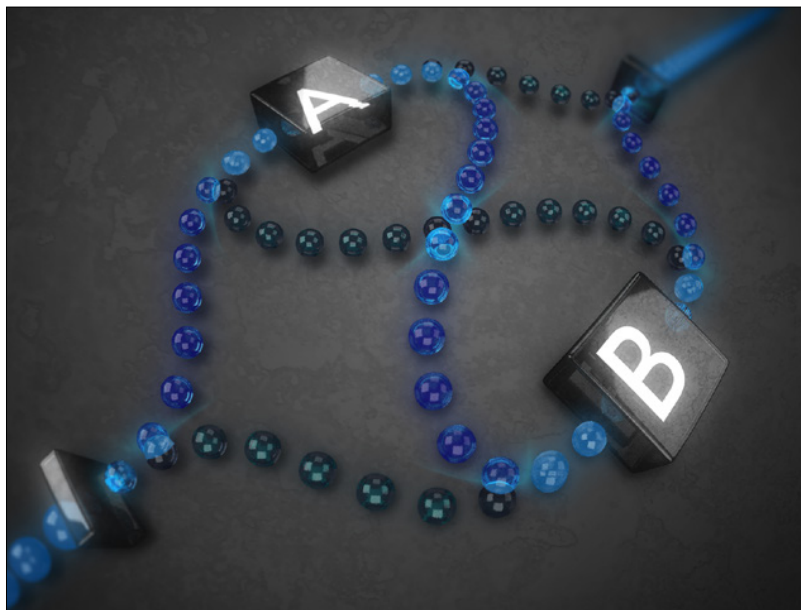


Illustration of superposition of quantum gates. Quantum mechanics does not only allow superposition of quantum states but also superposition of quantum gates. It was shown [1] that superimposing two quantum gates A and B, an unordered quantum computation can run more efficiently than a well-defined order quantum computation. The experimental demonstration was done in collaboration with the P. Walther group.

Quantum Information and Foundation of Physics (Zeilinger group)

Anton Zeilinger's group works experimentally and theoretically on fundamental tests of quantum physics and on their application to long-distance quantum communication. In 2015, the group was one of three internationally who performed a loophole-free test of Bell's inequalities [1]. This was followed in 2017 by tests of Bell's inequalities where the measurement settings for the two entangled photons were taken from Milky Way stars, putting any hypothetical common cause back by about 1.000 years, thus providing further evidence against any local realistic interpretation of quantum mechanics [2]. In parallel, a particular focus of the Zeilinger group is quantum phenomena in higher dimensions. This is aimed at extending the amount of information a single photon can carry. The work of these experiments is the orbital angular degree of freedom of light. We were able to show for the first time entanglement between more than two photons defined in more than two dimensions of Hilbert space. Furthermore, we have solved the question of what general quantum gates in high dimensions for single photons look like, and we were able to realize them in experiment. Most recently, we have performed the first experiment ever realizing GHZ entanglement between three particles beyond qubits. We also were able to realize novel tools for high dimensions, like entanglement of dimensions above 10.000, and ways to control polarization and coherence by the nonlocal Mandel effect.

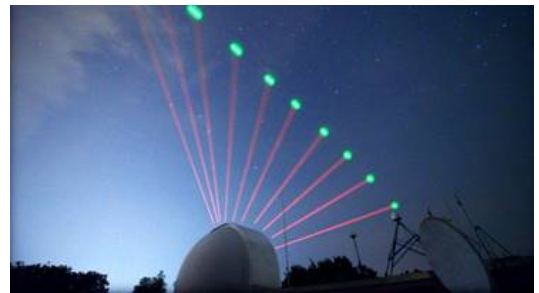
An experiment concerns Bose-Einstein condensation of metastable helium. We succeeded in putting the atoms in superpositions of well-defined momentum states and to outcouple small clouds of Bose-Einstein condensates. The next step is to demonstrate momentum entanglement, i. e. to realize the original Einstein-Podolsky-Rosen state. In another experiment, we have built up a single-photon source to study the response of single photoreceptor cells in retinas of toads and frogs.

One of the culminations of the last period was the successful establishment of a quantum cryptography link between China and Austria, using the Chinese quantum satellite Micius. That way, on 29 September 2017, the first intercontinental quantum cryptographically secured communication was possible.

In long-distance quantum communication, we implemented entanglement swapping, i. e. teleportation of entanglement between two Canary Islands, which is an important step towards future quantum repeaters. We also performed quantum communication with higher-dimensional OAM states, in Vienna over a distance of

3 km and again on the Canary Islands between La Palma and Tenerife over 143 km. Such experiments were theoretically predicted to be impossible due to the turbulence of the air. Recently, it was argued by another group that our experiments make it necessary to change the mathematical models of propagation of light in a turbulent atmosphere.

Some of the experiments in higher dimensions have been made possible by the new computer algorithm Melvin, which allows the automated search for new quantum experiments [3]. This learning algorithm was able to invent experimental setups which are far outside the reach of human intuition. It opened up the possibility for practical multi-photon entanglement, for cyclic transformation in higher dimensions, the development of novel single-photon quantum gates [4, 5] and of a new quantum router for higher dimensions. We also discovered an unexpected connection between quantum experiments and graphs [6].



Time lapse picture of satellite Micius passing the optical ground station (OGS) at Lustbühel. The OGS is pointing with a red uplink beacon laser towards the satellite. Once the satellite sees this beacon laser from the ground station it is sending infrared single photons for quantum key distribution together with a green downlink beacon laser for tracking back to the OGS.

Selected Publications

- [1] M. Giustina et al., **A significant-loophole-free test of Bell's theorem with entangled photons**, Phys. Rev. Lett. 115, 250401 (2015).
- [2] J. Handsteiner et al., **Cosmic Bell Test: Measurement Settings from Milky Way Stars**, Phys. Rev. Lett. 118, 060401 (2017).
- [3] M. Krenn, M. Malik, R. Fickler, R. Lapkiewicz and A. Zeilinger, **Automated Search for new Quantum Experiments**, Phys. Rev. Lett. 116, 090405 (2016).
- [4] A. Babazadeh et al. **High-Dimensional Single-Photon Quantum Gates: Concepts and Experiments**, Phys. Rev. Lett. 119, 180510 (2017).
- [5] M. Krenn, A. Hochrainer, M. Lahiri and A. Zeilinger, **Entanglement by Path Identity**, Phys. Rev. Lett. 118, 080401 (2017).
- [6] M. Krenn, X. Gu and A. Zeilinger, **Quantum Experiments and Graphs: Multiparty States as coherent superpositions of Perfect Matchings**, Phys. Rev. Lett. 119, 240403 (2017).

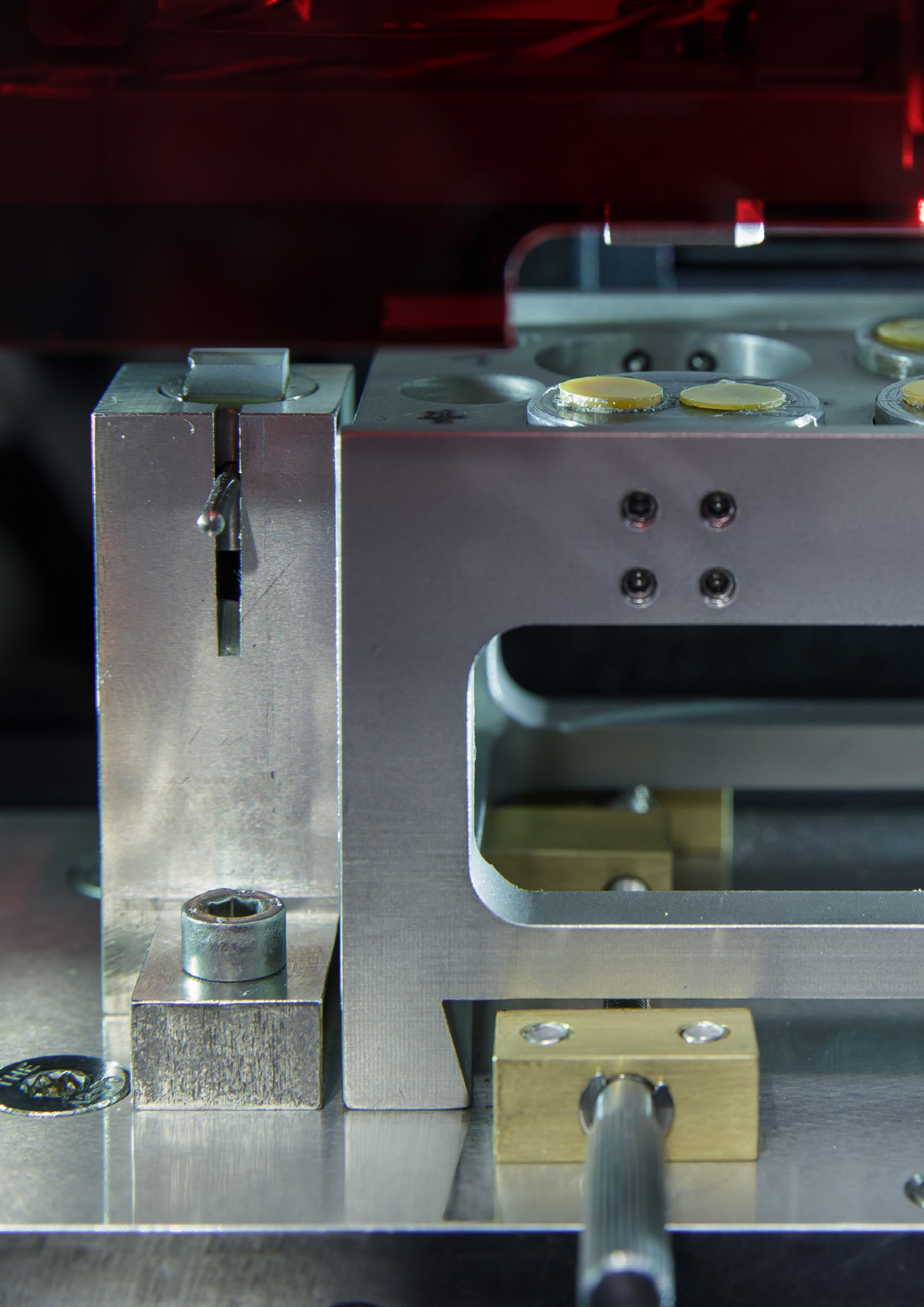
Workshop and Technical Services

The main task of the group is to manufacture mechanical parts and devices for the scientific research groups and for teaching purposes.

News

In 2016, a new 4-axis CNC milling machine was acquired as an extension of the existing machinery park. Due to the fourth axis (rotation axis) and the integration into the existing CAM system very complex parts can be produced. An automatic tool changer and an automatic tool measuring system make work easier and increase efficiency.







News and Outreach

Christian Doppler Laboratory – “Advanced Magnetic Sensing and Materials”

In May 2017 the Christian Doppler Laboratory “Advanced Magnetic Sensing and Materials” under the lead of Ass.-Prof. Dipl.-Ing. Dr. Dieter Suess started at the University of Vienna at the Functional Materials Group.

Research Topic

Within a cooperation between the University of Vienna, Danube University Krems and the industrial partners Infineon Technology AG and Magnetfabrik Bonn topics from 3D printing of magnets to the development of magnetic sensors are investigated.

Magnetic sensors are used in a wide range of applications, where robust, contactless sensing is required. For example modern cars contain several magnetic sensors to measure wheel speed, transmission gear speed and position, crankshaft position, engine speed, and much more. Currently a transition from the classical Hall effect sensors to GMR (Giant Magneto Resistance) and TMR (Tunnel Magneto Resistance) sensors takes place. Compared with classical sensors, magnetoresistive sensors offer enhanced sensitivity and thus extended range and applicability. Typical questions which are studied in cooperation with the commercial partner Infineon Technology AG include the effects of bias fields, surface roughness, sensor layout on the overall performance of the sensor. The final goal in sensor design is to reduce non-linearity, hysteresis as well as the magnetic noise of the sensor.

Due to non-linear and hysteretic effects like domain wall motion or switching events, the device modeling gets challenging. Fortunately the underlying physical processes can be well described by micromagnetic simulations. Sensor dimensions in the micrometer regime require very efficient numerical methods.

An example of a non-linear and hysteretic behavior is shown in Fig. 1 (a), where two consecutive passes of the hysteresis loop (red and green) are shown. For a reproducible sensor response, these loops should be identical. Within the Christian Doppler Laboratory a disruptive sensor technology is developed which realizes a topologically protected magnetic vortex state (Fig. 1 (c)) [1].

Compared to state-of-the-art sensors the proposed sensor layout has negligible hysteresis, a linear regime about an order of magnitude higher, and lower magnetic noise, making the sensor an ideal candidate for applications ranging from automotive industry to biological application.

The second main topic of the Laboratory deals with permanent magnets with the commercial partner Magnetfabrik Bonn. In commercial applications two main types of magnets exist that are sintered NdFeB magnets and polymer bonded magnets.

Within the Christian Doppler Laboratory for the first time commercial 3D printers were used to fabricate polymer bonded magnets [2,3]. The most important ingredient to transform a commercial 3D printer to a small sized magnets manufacturer is the filament which is usually a polymer. This polymer has to be replaced by a mainly magnetic material. In our case we use a compound of isotropic NdFeB particles inside a PA11 matrix which is extruded to filaments that is also a typical material used in polymer bond-

ed magnets. The used 3D printing system is also capable to extrude two different filaments, which allows a gradual change in magnetic properties. Hence, a continuous change from a magnetic material to a non-magnetic one can be realized as function of space. This capability allows generating magnetic field profiles which are not possible with other methods.

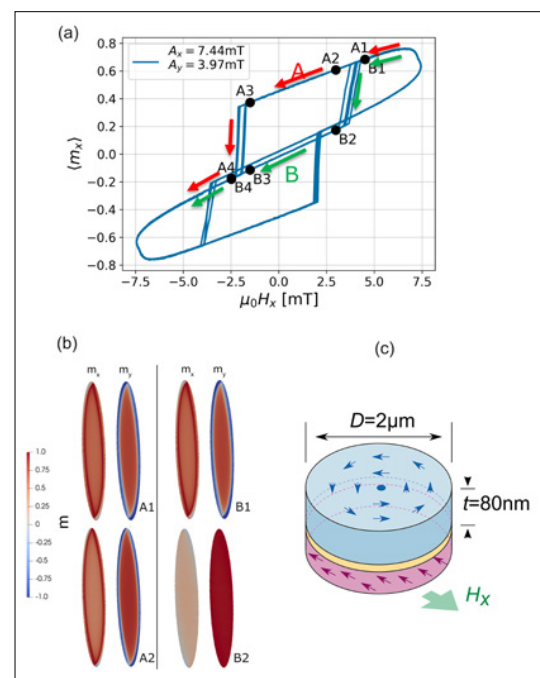


Fig. 1: (a) One magnetization component of the elliptical element of (b) as a function of the applied field H_x of a rotating field. Two consecutive passes of the hysteresis loop (marked red and green) show completely different behavior. (c) A topological protected vortex state is used in the sensing layer to avoid chaotic behavior of state-of-the-art sensors.

- [1] Zimmer, J., Satz, A., Raberg, W., Brueckl, H., & Suess, D. (2013). U.S. Patent Application No. 14/141,660.
- [2] Huber, C., Abert, C., Bruckner, et. al “3D print of polymer bonded rare-earth magnets, and 3D magnetic field scanning with an end-user 3D printer”, Applied Physics Letters, pp. 162401 (2016).
- [3] The Economist, “Additive manufacturing – Magnetic moments” pp. 68, Nov. 19th – 25th (2016).

Christian Doppler Laboratory for Semiconductor Optics and Mid-IR Spectroscopy



Figure 1: The CDL team as of January 2018

The research in the Christian Doppler Laboratory for Mid-IR Spectroscopy and Semiconductor Optics covers all aspects of cavity enhanced frequency comb spectroscopy in the mid-infrared (mid-IR).

We strive to extend frequency comb technology further into the mid-IR spectral region and pursue applications with these frequency combs in the field of trace gas detection, precision spectroscopy and molecular fingerprinting.

Progress in the mid-IR spectral region has been hindered in large part by the lack of high quality and low loss optics. Within the Christian Doppler laboratory, we will explore the advantages and possibilities of newly available high reflectivity and low loss optics in the mid IR. These revolutionary mirrors are based on crystalline supermirror technology provided by our industrial partner Crystalline Mirror Solutions.

Crystalline Mirrors

Highly reflective optical interference coatings are indispensable tools for modern scientific and industrial efforts in photonics. Systems with ultra-low optical losses, namely, parts per million (ppm) levels of scatter and absorption, were originally developed for the construction of ring-laser gyroscopes by Litton Systems in the late 1970s. Stemming from this breakthrough, ion beam sputtering (IBS) is now firmly established as the gold standard process technology for generating ultralow-loss reflectors in the visible and near infrared (near-IR).

Though exhibiting phenomenal optical properties, limitations of these amorphous coatings include excess Brownian noise, negatively impacting the ultimate performance of precision optical interferometers, poor thermal conductivity, as well as significant levels of optical absorption for wavelengths beyond $2\ \mu\text{m}$.

Crystalline interference coatings offer vastly reduced Brownian noise, the highest thermal conductivity (about 30 times higher than conventional mirrors) and achieve optical performance that rivals those of IBS multilay-

ers in both the near-IR and mid-IR.

We fully characterize mid-IR mirrors, which includes their reflectivity, transmission and losses (scatter and absorption) as well as their group delay dispersion. Together with CMS we work on new and perfected mirror designs.

Mid-IR Frequency Combs

Mid-IR frequency combs have emerged as a new generation of spectroscopic tools for molecular science due to their ability to quickly acquire a broadband molecular spectrum with high spectral resolution. High average power frequency combs allow for increased sensitivity and shorter acquisition times. Our work on frequency combs focuses on increasing the average output power of mid-IR frequency combs and extending the wavelength coverage further into the mid-IR spectral region.

Frequency Comb Spectroscopy

Mid-IR frequency combs enable detection of molecular species showing absorption in the important molecular fingerprint region between $500\ \text{cm}^{-1}$ and $4000\ \text{cm}^{-1}$ ($2.5\text{--}20\ \mu\text{m}$). Examples include the detection of pollutants such as ozone, methane, carbon monoxide, nitric oxide or biomarkers indicating malignoma or other severe diseases. Our current research focuses on high spectral resolution frequency comb spectroscopy.

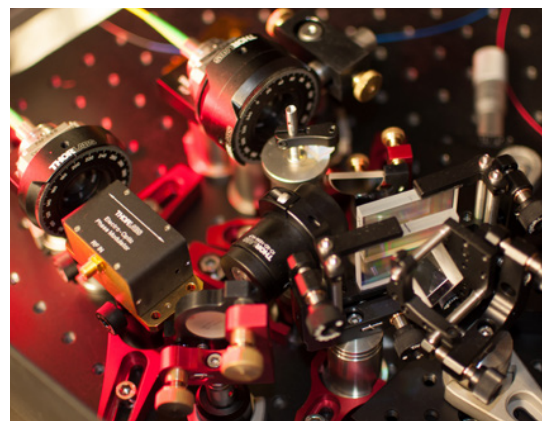


Figure 2: Early stage frequency comb

Research Platform TURIS

The two main pillars of modern science are the theories of general relativity and quantum mechanics. These two theories are fundamentally different: quantum mechanics allows for a description of nature at the small scale, whereas general relativity gives access to descriptions at the very large scale, up to cosmological distances. In 2017 the research platform “Testing quantum and gravity interface with single photons (TURIS)” was founded at the University of Vienna. Its goal is to investigate up to which extent foundational principles of the two theories are compatible with each other. This may open new perspectives on how to best reassess already known challenges in the development of a complete theory unifying quantum theory and general relativity.

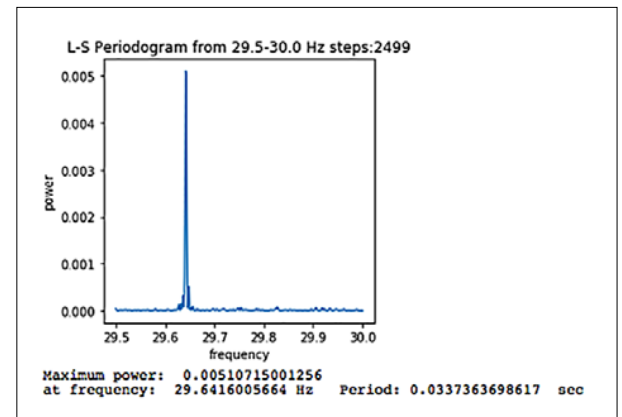
TURIS aims to use and combine the unique experimental framework existing at the Faculty of Physics and at the Department of Astrophysics for designing sensitive quantum experiments ranging from various table-top experiments using photons (Prof. Philip Walther), matter waves (Prof. Markus Arndt), nano-mechanical devices (Prof. Markus Aspelmeyer) to large-scale experiments using satellites (Prof. Joao Alves). These efforts will be accompanied by theoretical studies on the quantum description of the influence of gravity (Prof. Piotr Chrusciel) and its quantum physics signatures (Prof. Caslav Brukner).

Already within the first year of TURIS various scientific results have been achieved: In collaboration with the University of Florence we reported on a novel Weak Equivalence Principle test for atoms. In addition we could show that since any quantum clock must be in a superposition of energy eigenstates, the mass–energy equivalence leads to a trade-off between the possibilities for an observer to define time intervals at the location of the clock and in its vicinity. In collaboration with LIGO-MIT we analysed and proposed an experimental setup for measuring the gravitationally induced phase-shift on a single photon.

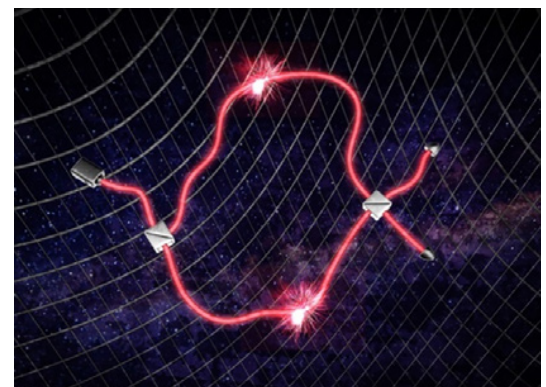
During 2017 a fast photometer to be used by TURIS to study signal attenuation by the atmosphere towards a TURIS experiment involving satellites, was designed and built for the 1.5 m Figl telescope of the University of Vienna, located in the Vienna forest (Schöpfl mountain). The instrument reached “first-light” on October 30th with the observation of the Crab pulsar (see light curve below). Work is still ongoing to finish and calibrate the instrument but the successful “first-light” was an important milestone in 2017.

Selected Publications

- [1] Gravitationally induced phase shift on a single photon
C. Hilweg, F. Massa, D. Martynov, N. Mavalvala, P.T. Chruściel, P. Walther,
New Journal of Physics 19, 033028 (2017).
- [2] G. Rosi, G. D’Amico, L. Cacciapuoti, F. Sorrentino, M. Prevedelli, M. Zych, Č. Brukner, and G. M. Tino,
Quantum test of the equivalence principle for atoms in coherent superposition of internal energy states, Nature Communications 8, 15529 (2017).
- [3] I. Pikovski, M. Zych, F. Costa, Č. Brukner,
Time Dilation in Quantum Systems and Decoherence, New J. Phys. 19, 025011 (2017).
- [4] E. Castro, F. Giacomini, Č. Brukner,
Entanglement of quantum clocks through gravity,
doi: 10.1073/pnas.1616427114, PNAS March 7 (2017).



Lomb-Scargle periodogram of the “first-light” data, pointing to the canonical 33 millisecond period.



Artistic scheme of a Mach-Zehnder interferometer for observing gravitational effects on a single photon whose superimposed position is affected by gravity.

The Vienna Doctoral School in Physics (VDS-P)



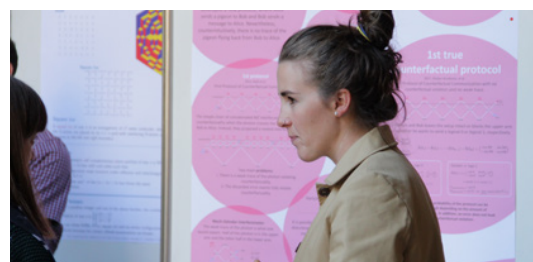
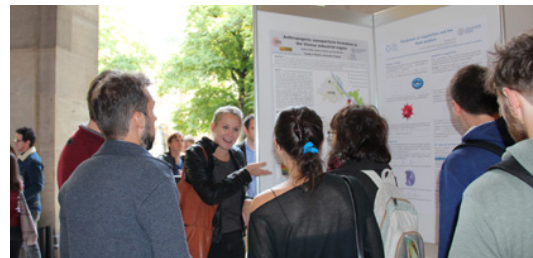
“Physics Meets: Science and the Public“



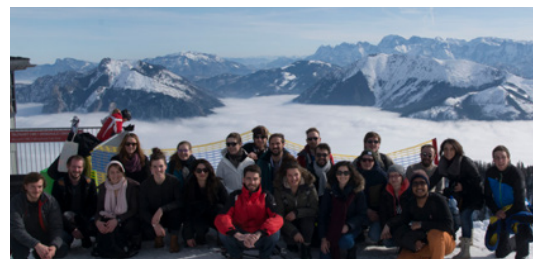
Picture 1: On 26 January 2017 the VDS-P event "Physics Meets: Science and the Public" took place at the Erwin Schrödinger Institute in Vienna.

The VDS-P program, headed by Prof. Markus Arndt, offers research opportunities in 21 different research groups working in experimental, theoretical or computational physics. It is the first structured doctoral program at the University of Vienna across the entire Faculty of Physics, selecting and supporting the young researchers in a joint effort. At the end of 2017 the VDS-P consisted of 35 fellows dedicated to excellence in research and engaged in networking activities.

In 2017 these activities included two panel discussions with distinguished guests from politics, science and industry – together with VDS mathematics –, a winter retreat in the alps, an interactive science communication course, and the first interdisciplinary symposium between the four schools on “Cognition, Behaviour and Neuroscience”, “Mathematics”, “Molecules of Life” and “Physics”. VDS-P enabled the active participation of our promising young researchers in international conferences as well as their outreach activities.



Picture 2 & 3: On 14-15 September 2017 the symposium organized by all four VDSs took place. These two photos were taken in the Arcadenhof during the poster sessions.



Picture 4: In February 2017 the VDS winter retreat took place in Upper Austria.



Picture 5 & 6: The winter retreat in February 2017. These photos were taken during the Arduino workshop.

Science Outreach

In 2015, the University of Vienna celebrated its 650th anniversary and opened its doors to the public to provide information about the University's responsibilities and achievements. The Faculty of Physics organised and participated in various events to highlight the importance of research and teaching in advancing our society and educating future generations.

University of Vienna Campus Festival

A highlight among the activities for the 650th anniversary of the University of Vienna was the three-day Campus Festival that took place from June 12-14, 2015. The Faculty of Physics offered 9 interactive research stations and participated in the research rally, the children's programme ("Fun with Physics"), the event "Uni:Orientiert" (information event for high school students), Future Lab, a competition for high school students, and in public lectures. Faculty staff and students presented their research in experiments, videos and one-on-one talks. From Friday to Sunday, the Campus Festival saw a total of 33,000 science enthusiasts who visited the multifaceted presentations of research highlights.

Fascinating Physics – A Day to Experiment and Discover

During the Faculty's "Open Day" on June 19, 2015 we offered a varied programme for interested students, grown-ups and children of all ages.

[physics:open 2015 for school classes](#)

Our tried and tested info event for students from grade 7 and up allowed for insights into physics and research via numerous exciting experiments and interactive presentations.

Visiting the physics labs

Where are bright ideas put into practice? What do research labs look like in which new insights into the fundamentals of science are gained? Which technologies are used? Young scientists gave half-hourly tours of the labs of the Faculty of Physics and explained on location which exciting experiments they are using to research open questions of science from environmental physics and isotope research to materials science and quantum physics.



On the Shoulders of Giants – The Historical Collection

Tours through the Historical Collection of the Faculty of Physics gave visitors an opportunity to marvel at selected highlights among the ~ 1000 measuring instruments and teaching objects, some of which had already been used by famous Viennese physicists like Christian Doppler and Josef Stefan around 1850.

Physics Soiree

Multimedia lectures in gravitational physics, materials physics, aerosol physics and quantum physics allowed visitors to gain an insight into fascinating research topics at the Faculty of Physics. Current findings and open questions were discussed.

Einstein on Tour

In the interactive exhibition “Einstein on Tour”, our guests were able to ride a bike at almost the speed of light, to fly through an island landscape in a fast-paced simulation, or to experiment with a black hole. This allowed them to explore Albert Einstein’s theories of relativity in a playful manner.

Taster lab course Physics

Why is spinach green? How do criminologists identify unknown substances? Interested visitors discovered the answers for themselves through experiment, and got to experience what being a physics student in the physics lab course feels like.

Hands-on experiments for young scientists

In the student teachers’ lab young participants were able to experience fun and thought-provoking experiments first-hand.

Women physicists in 20th century Vienna

A permanent exhibition showcases the lives and works of important women physicists of the interwar and postwar periods. The accompanying video presentations “A Retrospective of Physics in Vienna – Recollections by Contemporary Witnesses”, developed in cooperation with the Austrian Central Library for Physics, introduce a great figure of Viennese University history – Prof. Berta Karlik – and offer a glimpse into what studying and researching was like at the time.

Behind the Scenes – the Workshop

The Workshop and Technical Services team supports the research groups by fabricating specialised devices and construction elements. During the Open Day, visitors were given the opportunity to examine the excellent technical equipment: metal cutting, sheet metal forming, welding and



electronics for high-tech experiments at the forefront of research.

The Knowledge of Things – An Exhibition at the Natural History Museum Vienna

The anniversary exhibition examines university-level teaching and research in the natural sciences over the previous 250 years. The Faculty of Physics displays selected exhibits, interactive experiments and multimedia contributions:

18th Century Physics Teaching – Mechanical Objects

Selected 18th century classroom demonstrations that are part of the Historical Collection of the Faculty of Physics (curator: Ass.-Prof. Dr. Franz Sachslehner) bore witness to the teaching practice of times past: an Archimedean screw, presented to the University of Vienna by the Habsburg Art Collection in 1790, an Atwood machine and mechanical models made of wood that presumably trace back to Joseph Walcher.

Physics Teaching Today – The Virtual Quantum Lab

An interactive research simulation developed by PhD student Mathias Tomandl from Prof. Markus Arndt’s Quantum Nanophysics group simulates an up-to-date quantum physics lab at the Faculty of Physics. It is used in teaching at the University of Vienna and can be accessed on the internet by anyone who is interested.

Physics Research Today – Modern Spectroscopy

A multimedia presentation showed how researchers from Prof. Thomas Pichler’s Elec-

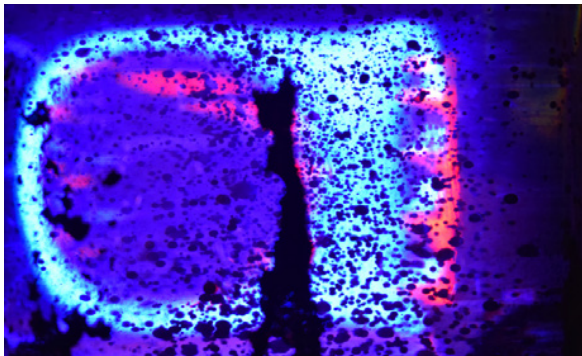
tronic Properties of Materials group devise a “fingerprint” of novel materials via cutting-edge spectroscopy.

Physics Research Today – Modern Microscopy

Videos and microscope images from Prof. Jannik Meyer’s UltraSTEM Lab (Physics of Nanostructured Materials group) accompanied visitors into the world of atoms and let them experience how researchers at the Faculty of Physics use one of the best electron microscopes worldwide to zoom into matter and gain knowledge about innovative materials.

“The Art of Magnetism”

The science communication project “The Art of Magnetism” funded by the Austrian Science Fund FWF brought the cutting-edge research on dipolar soft matter of Sofia Kantorovich’s FWF START project “Bridging Scales in Dipolar Soft Matter” to a wider audience. Throughout 2016, “The Art of Magnetism” took advantage of Vienna’s cultural and artistic traditions to make the soft matter research more visible and accessible through exhibitions with interactive artworks, workshops and public lectures organised in collaboration with artists. The researchers sparked curiosity for magnetic materials and scientific approaches in various groups of different age, gender, nationality and educational background following an interdisciplinary concept. Additionally, the presence of artists facilitated the dialogue between lay people and scientists. Impressions of the activities of the project “The Art of Magnetism” can be found on the project’s website: <https://artofmagnetism.wordpress.com/>



Future Lectures 2017

Under the patronage of Dennis Meadows (Pioneer of Growth Criticism), teams of teachers and students organise FUTURE LECTURES together with the FORUM Environmental Education at three universities or colleges each year. In these exciting trilogies, current opportunities, challenges and contradictions of sustainable development are discussed beyond interdisciplinary borders. On December 14th, the 3rd FUTURE LECTURE 2017 took place at the Faculty of Physics, University of Vienna, on the basic question “Physics + Technology -> Sustainability?”. Experts of the Faculty of Physics from the fields of Aerosol Physics (Univ.-Prof. Dr. Bernadett Weinzierl) and Computational Material Physics (Assoz. Prof. Dr. Kerstin Hummer) as well as from the technical and application-oriented area (Dr. Marcus Rennerhofer, Austrian Institute of Technology) and the field of education (Dipl.-Ing. (FH) Martin Striok, HTL Hollabrunn) gave impulse lectures on the extent to which research in the field of physics, developments in photovoltaics and the role of education contribute to sustainability. Using an online tool, participants were able to ask the lecturers questions at any time. Together with the lecturers, a bridge between science, teaching and practice was successfully built.



Frequent outreach activities

As part of its public outreach mission, the Faculty of Physics offers a diverse range of activities for people of all ages, for the general public and for groups with a particular interest in physics. The various activities take place throughout the academic year and guarantee a continuous and exciting programme.

Every year, members of the Faculty of Physics take part in the Vienna Children's University (Wiener Kinderuni) organised by the Vienna University Children's Office (Kinderbüro der Universität Wien). In 2017 more than 500 children attended 12 diverse courses, workshops, excursions and interdisciplinary seminars which were led by more than 20 faculty members. In two further activities initiated by the Vienna University Children's Office, the Kinderuni on Tour and the UniClub, respectively, a university lecturer was assisted in a real open-air lecture by children conducting small experiments and a tailored programme was offered to high school students from disadvantaged backgrounds in order to get informally in contact with higher education.

In 2017 it was already the eighth time that the Faculty of Physics organised, in collaboration with the Vienna School Board, "physics:science@school", a series of lectures for particularly interested high school students aged 16 to 19. In 18 events spread over the last two years more than 1,000 students and teachers were able to attend the lectures in various host schools given by researchers of the Faculty of Physics.

Further yearly activities include the weekly guided tours at the VERA laboratories, interactive workshops within the course of the "Junior Science Club" in cooperation with the Vienna School Board, summer internships for young adults in cooperation with the Austrian Research Promotion Agency (FFG) financed by the Austrian Ministry for Transport, Innovation and Technol-

ogy (bmvit) as well as taster lectures and lab courses in the scope of Uni:Orientiert, the annual information event on study options at the University of Vienna.

The Faculty of Physics also invited female high school students to experience first-hand how exciting and versatile higher education in natural sciences and engineering can be by tailoring workshops for the programmes "FIT – Frauen in die Technik" and "Wiener Töchtertag".



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Clemens Nagel; Daria Setman

Imprint

Publisher

Faculty of Physics
Boltzmanngasse 5
1090 Wien, Austria
<https://physik.univie.ac.at>

Visual design

Elisabeth Frischengruber