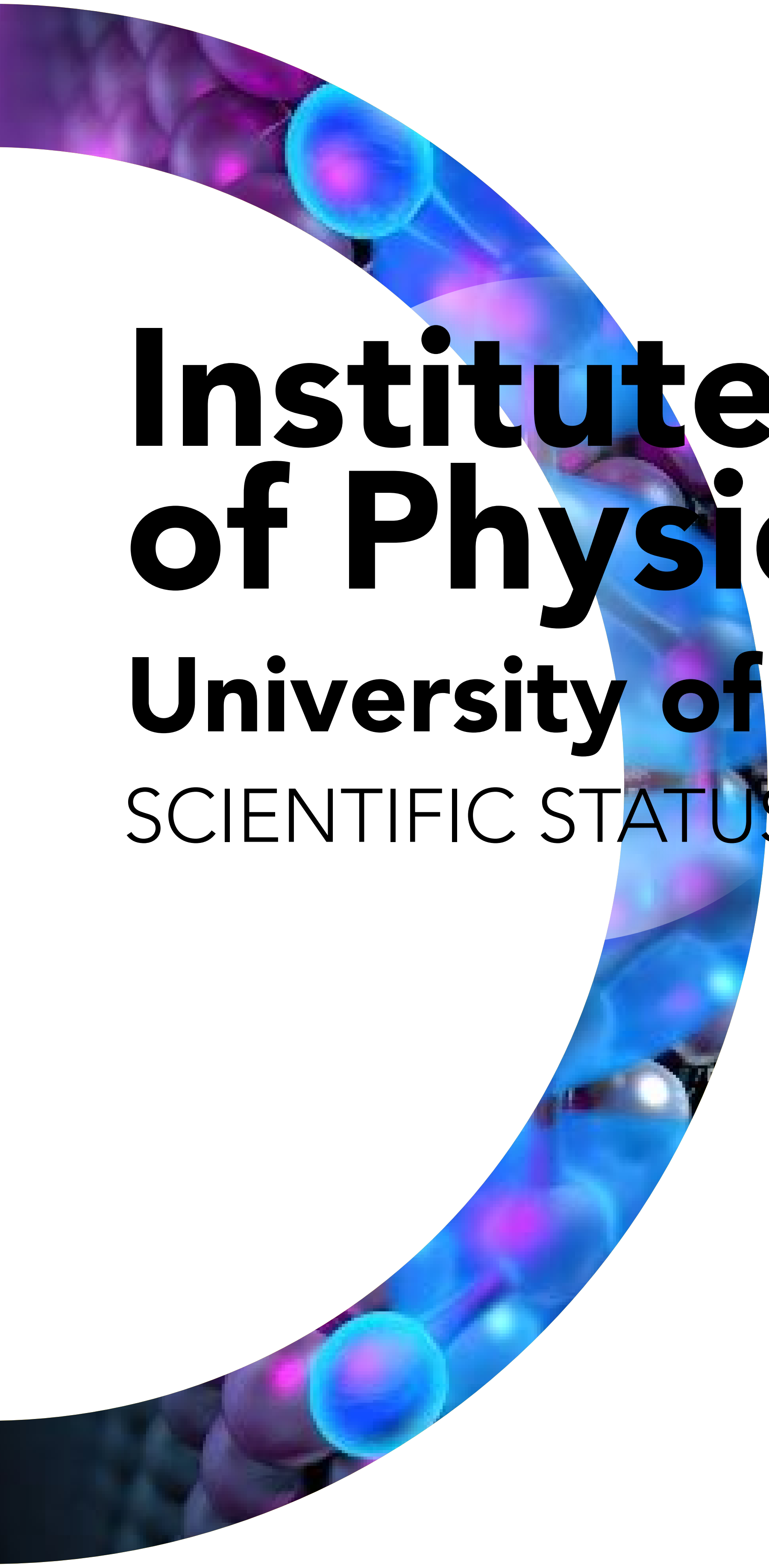

Institute of Physics

University of Graz

SCIENTIFIC STATUS REPORT

We work for **tomorrow**

www.uni-graz.at

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Intro-duction

Physics in Graz, and especially at the University of Graz, has a long, highly successful, and illustrious history. Especially in the last decades, this history was signified by becoming a more and more unified structure while at the same time retaining the ability to represent the full breadth of modern physics in teaching, research, and the education of future teachers of physics. This was signaled by the formation of one common institute and the cooperation with the Technical University of Graz in NAWI physics. It will find its logical conclusion within the decade by the founding of the Graz Center of Physics (GCP), which will unify in one entity all of university physics in Graz.

The document you are reading forms an important step in this process. It takes an overall look of the recent achievements of the Institute of Physics at the University in Graz, especially in the years 2018-2020 during which the plans for the GCP took its current shape. At the same time, it sketches the future strategy for the first half of the common transition period into the GCP: What are the scientific areas to be covered and the measures to implement them. It focuses on the research activities, and is thus organized around the individual research groups. The institute's work is supported by an excellent administrative staff and technical staff, whose support is invaluable for the smooth running of the research.

The next report will be prepared in 2024 and it will document how these strategies have been implemented, and how the necessary adaptation to new scientific insights in this period have been realized. As scientific research is always changing, can only be - and are - the based on our current knowledge.

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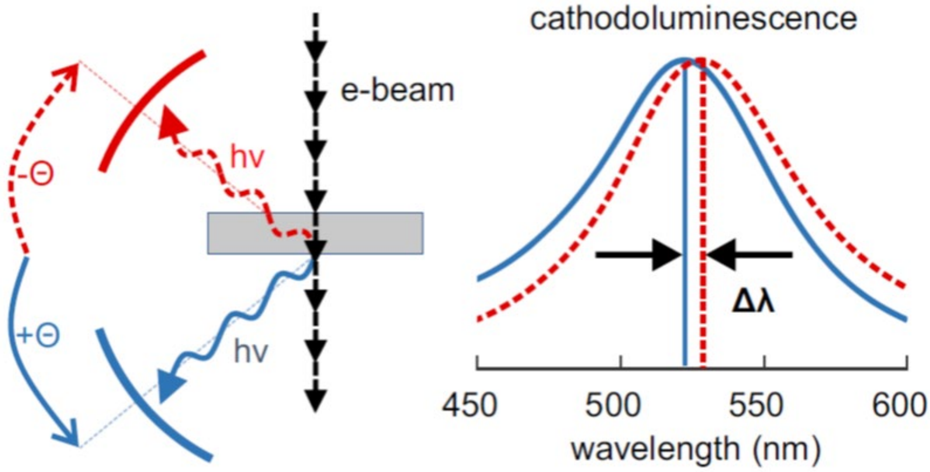
An ultimate limit



Left: Light emitted upon the interaction of a tightly focused electron beam is detected in backward and forward direction. Right: A shift in the peak maxima of the backward and forward spectra is observed.

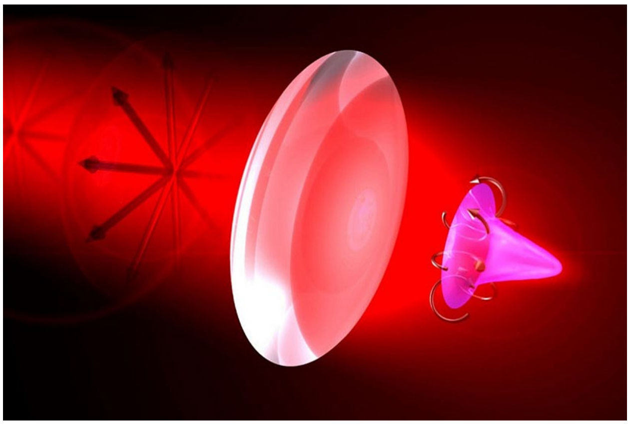
Optical measurements with an electron beam: What seems contradictory at first glance is a method in which the light emission of a sample excited by electrons is measured. The advantage: The electron beam can be focused down to atomic dimensions, resulting in a spatial resolution that is many times higher than that of excitation with light.

This "cathodoluminescence" method has been used in the most advanced electron microscopes in recent years to research optical nanostructures with ever greater precision. This naturally also gave rise to the question of the limits of the method, a question that two research groups from the Institute of Physics have now answered in collaboration with groups in Vienna, the Czech Republic and France.

The cooperation project investigated so-called plasmons in disk-shaped nanoparticles made of silver. Initially, there were inexplicable systematic differences in the spectral position of the maximum luminescence that were dependent on the direction of emission. Comparing the experimental results to numerical simulations finally solved the riddle: The break in symmetry caused by the direction of the electron beam leads to different charge densities on the two particle surfaces – and this to a direction-dependently modified light emission. Although the spectral differences are only a few nanometers, understanding them as a phenomenon caused by the exciting electron beam itself is of central importance: This is the only way to correctly interpret future precession measurements.

Franz-Philipp Schmidt, Arthur Losquin, Michal Horák, Ulrich Hohenester, Michael Stöger-Pollach, Joachim R. Krenn, Fundamental Limit of Plasmonic Cathodoluminescence, Nano Letters 21, 590-596 (2021) https://doi.org/10.1021/acs.nanolett.0c04084

Light keeps spinning



Polarizing light and making it spin by focussing.

In collaboration with teams from the UK, Japan, France and the US, researchers at the University of Graz and the Max Planck Institute for the Science of Light have shown that you not always have to use polarization optics to polarize light. They prove that via spatial confinement, fully unpolarized light can be polarized circularly.

One of the most intriguing features of electromagnetic waves in general and light in particular is their polarization. It defines how the electric field component of an electromagnetic wave is oriented and changes with time. If the electric field oscillates in a fixed plane, the wave is said to be linearly polarized while a field spinning about an axis – usually the propagation direction of the light wave – is circularly or elliptically polarized. The rotational dynamics of elliptically or circularly polarized light also give rise to an intimately related property, the so-called spin (angular momentum). Just like the propeller of an airplane, also the spinning electric field of light carries angular momentum. Naturally and quite intuitively, if light is totally unpolarised, just like the light coming from a light bulb or LED, the polarization is not defined and also its spin should vanish.

About a decade ago, members of the aforementioned international teams discovered that light might also behave like a spinning wheel, i.e., the angular momentum can be orthogonal to the propagation direction of a light wave with the field spinning in the propagation plane, just like the spokes of a wheel. Originally considered as an exotic and exclusive phenomenon, it was shown by the authors and their colleagues that this feature of so-called *transverse spin* is a ubiquitous feature arsing in various schemes involving spatial confinement of light.

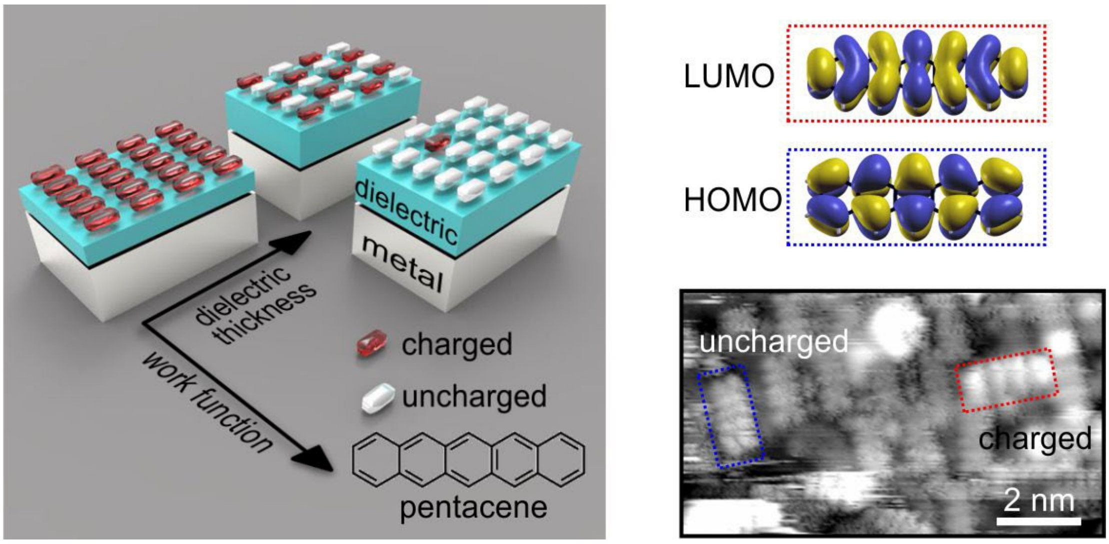
In a collaborative project, the international teams now brought together these two concepts of unpolarized light and transverse spin in two conceptually quite different experiments and a unified theoretical framework. Counter-intuitively they showed that fully unpolarised light beams can be polarized circularly and feature non-zero (transverse) spin by simple spatial confinement. This is a remarkable finding because it would allow for polarizing light and making it spin by, e.g., simple focusing, which seems to contradict the simple and established understanding of spin and polarization of unpolarised light. Key to this discovery is the intricate structure of light at micro- and nanoscale and the ubiquity of transverse spin. This international collaboration sheds new light on the properties of unpolarized waves and fields, opening up a whole new avenue for the implementation of polarization-sensitive experiments in various areas of optics.

J. S. Eismann, L. H. Nicholls, D. J. Roth, M. A. Alonso, P. Banzer, F. J. Rodríguez-Fortuño, A. V. Zayats, F. Nori, K. Y. Bliokh, *Transverse spinning of unpolarized light*, Nat. Photon. 15, 156-161 (2021); *https://doi.org/10.1038/s41566-020-00733-3*

Nature Photonics News & Views: https://www.nature.com/articles/s41566-020-00756-w

News article on PhysicsWorld: https://physicsworld.com/a/spin-in-unpolarized-light-defies-conventional-picture/

Charge makes the difference



Left: Schematic illustration of the influence of work function and dielectric thickness on the charging of pentacene molecules on ultrathin magnesium oxide films supported on Ag(001). Right: Calculated orbital structures of the lowest unoccupied (LUMO) and highest occupied (HOMO) molecular orbital of a pentacene molecules. Scanning tunneling microscopy image of a monolayer pentacene on high work function MgO(001)/Ag(001) showing the coexistence of integer charged and uncharged pentacene molecules.

Ultrathin dielectric layers can be found in many technologies ranging from catalysis to organic electronics. Their presence (whether intentional or unintentional) can have profound influence on the chemical and electronic properties of a material. For example, it has been shown that ultrathin dielectrics on metals can reduce the work function of the metal such that charge transfer via tunneling through the dielectric layer into adsorbed atoms or molecules becomes possible, which might have strong effect on the surface reactivity, magnetic moments and charge injection at the contacts of organic devices. Whether this charge transfer occurs in integer units of electronic charge or not, and how the potential equilibration at the interface is accomplished, has long been a matter of debate and remained elusive from an experimental point of view.

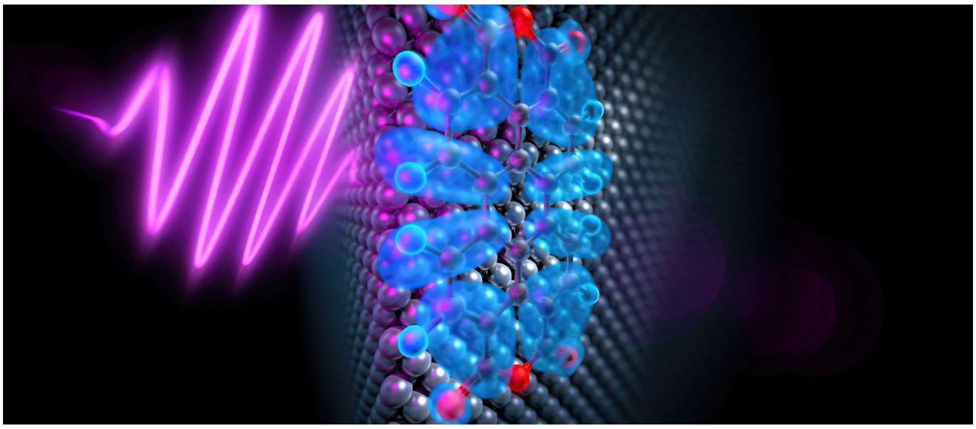
The team around Michael G. Ramsey, Martin Sterrer and Peter Puschnig from the Institute of Physics could demonstrate with a combined experimental and computational work on a model system (ultrathin MgO films on Ag(100) with adsorbed pentacene molecules) that the charge transfer process and the potential equilibration is governed by the proportion of integer charged and uncharged molecules. Moreover, they could show that the ratio of charged and uncharged molecules can be controlled by either tuning the work function of the substrate or the thickness of the dielectric, confirming that the process can be understood and explained with a simple capacitor model. The understanding gained in this work demonstrates how charge transfer in such systems is controlled and paves the way for tuning their chemical and electronic properties in desired directions.

P. Hurdax, M. Hollerer, P. Puschnig, D. Lüftner, L. Egger, M. G. Ramsey, M. Sterrer

Controlling the charge transfer across dielectric interlayers.

Adv. Mater. Interfaces, 2020, 7, 200592. https://doi.org/10.1002/admi.202000592

Electron and phonon dynamics in time and space



A laser pulse excites an electron from a molecular orbital, © Till Schürmann, Philipps-Universität Marburg.

The solid-state theory group investigates interactions of light and electrons with solid-state nanostructures. The topic is of great importance for understanding and optimizing chemical reactions on surfaces, intermolecular charge transfer, and light confinement and heat transfer at the nanoscale, which will impact the development of novel concepts for energy storage and light harvesting.

In early 2021 two papers have been published in the renowned Science journal and have been highlighted there as follows:

R. Wallauer et al., Tracing orbital images on ultrafast time scales, Science 371, 1056 (2021).

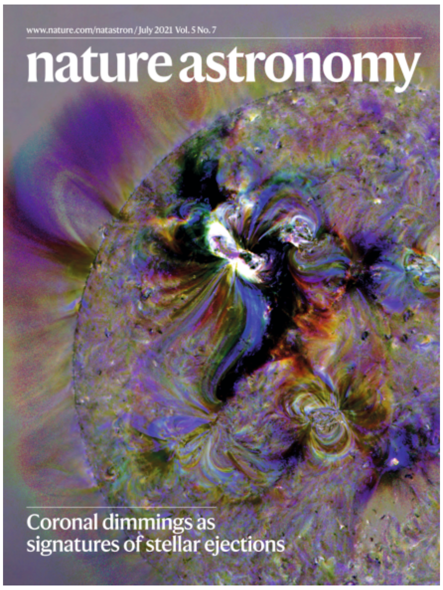
Following molecular excitation and electron transfer processes in time and space within a single experiment is a long-standing goal of spectroscopy in the field of chemistry. Wallauer et al. combined tomographic photoemission imaging with a femtosecond pump-probe scheme to trace the excited state molecular orbitals of surface-adsorbed molecules with both spatial and temporal resolution. The present demonstration opens a new window for investigating the ultrafast electron transfer dynamics in such processes as chemical reactions on surfaces and intermolecular charge transfers.

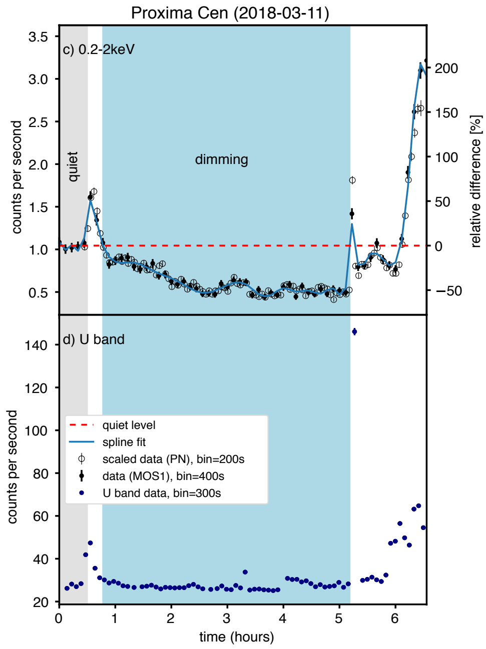
X. Li et al., 3D vectorial imaging of surface phonon polaritons, Science 371, 1364 (2021).

Atomic vibrations (phonons) govern many physical properties of materials, especially those related to heat and thermal transport. They also provide fingerprints of the chemistry of a wide variety of materials, from solids to molecules. The behavior of phonons in nanostructures can be appreciably modified because of confinement effects. Li et al. combined several electron microscopy techniques to map out the phonon-polariton excitations across the surface of magnesium oxide nanostructures with high spatial, spectral, and angular resolution. The reconstruction of the surface excitation maps in three dimensions will be useful for understanding and optimizing the properties of the nanostructured materials for advanced functionality.

Peter Puschnig and Ulrich Hohenester from the solid-state theory group have contributed to these studies through various Schrödinger and Maxwell simulations for interactions of electrons and light with nanostructures. All members of the group are well embedded in numerous national and international collaborations. The simulation of nanostructures will be of pivotal importance for the core areas “Nano and quantum materials” and “Computational Physics” of the future Graz center of physics.

New detection method for stellar mass ejections





Left: Coronal dimmings (dark areas) caused by a massive coronal mass ejection from our Sun. The image combines observations of three filters at extreme-UV wavelengths by the Atmospheric Imaging Assembly (AIA) sensitive to different temperatures of the solar corona. Right: Coronal dimming detected on our nearest neighbor star, Proxima Centauri. The drop of the X-ray counts after the flare enhancement recorded by XMM-Newton is indicative of a stellar mass ejection. From Veronig et al., Nature Astronomy 5, 697-706 (2021).

Coronal mass ejections (CMEs) are huge expulsions of magnetized matter from the Sun and stars, traversing space with speeds of millions of kilometres per hour. Solar CMEs can cause severe space weather disturbances and consumer power outages on Earth. Stellar CMEs may even pose a hazard to the habitability of exoplanets the star is hosting. CMEs ejected by our Sun are regularly imaged by white-light coronagraphs, and their speeds and masses are derived from these observations. However, for stars such direct imaging is not possible, and so far, only a few candidates for stellar CME detections have been reported. In a recent study published by Veronig et al. in the July 2021 issue of Nature Astronomy and featured on the journal cover, we demonstrated a new approach that is based on sudden dimmings in the extreme-UV and X-ray emission caused by the CME mass loss. This study resulted from a joint endeavor of the solar and astrophysics research teams at Uni Graz.

Sun-as-a-star broad-band EUV light curves were used as a testbed to study whether coronal dimmings can be also observed on stars and used for stellar CME detection. The study demonstrated that large eruptive flares are with a high probability associated with a post-flare coronal dimming, with intensity drops in the 15-25 nm full-Sun light curves up to 5%. Searching for similar patterns of post-flare dimmings in the X-ray and EUV light curves of solar-like and late-type stars, 21 stellar CME candidates were identified, which is more that all previous reports of stellar CMEs. The derived intensity drops are an order of magnitude larger than for the Sun, suggesting that a substantial part of the stellar corona gets ejected by the CME. This study paves the way for comprehensive detections and characterizations of CMEs on stars, which are important factors in planetary habitability and stellar evolution.

A.M. Veronig, P. Odert, M. Leitzinger, K. Dissauer, N. Fleck, H.S. Hudson, Indications of stellar coronal mass ejections through coronal dimmings, Nature Astronomy 5, 697-706 (2021). https://www.nature.com/articles/s41550-021-01345-9

Didactics

Design-Based Research for instructional innovations in physics teaching and learning

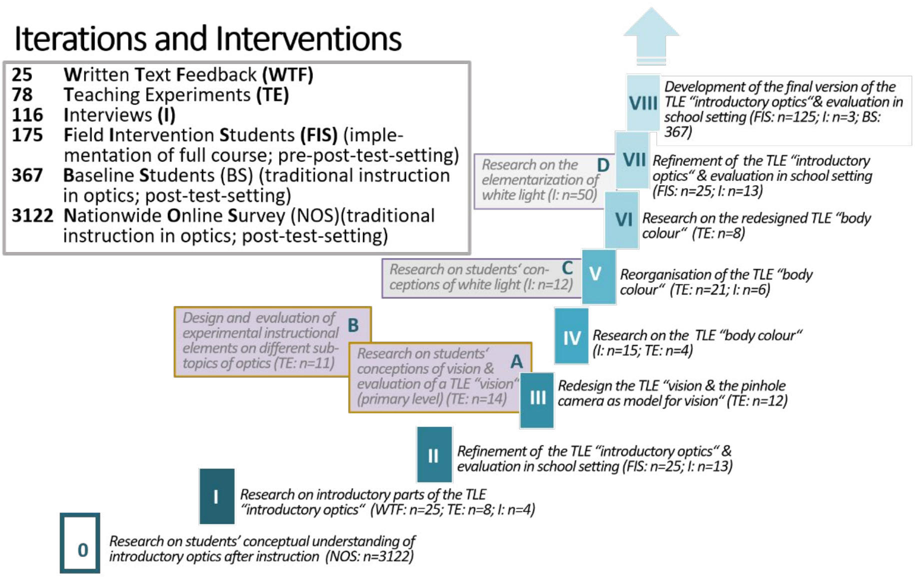
Lately, the Physics Education Research Group has substantially contributed to curriculum design and the further development of Design-Based Research. DBR usually starts from practical problems and produces in iterative cycles of analysis, design, empirical testing and redesign, curricula and materials for practice. Simultaneously, domain specific instruction theories and design-knowledge are generated.

Analysing traditional teaching as starting point – introductory electricity

Electricity is difficult for most lower-secondary students, especially the development of an adequate conceptualisation of voltage. PER has identified several instructional components like the choice of content structure, meaningful elementarisation of basic concepts or adequate use of analogies that support the development of students' conceptual knowledge. For the theory-lead and research-based development of curricula (eg. EPo-EKo-Project), empirical insights into the common teaching practice are necessary. Our analysis of four widely used physics school textbooks[1], the analysis of introductory electricity lessons as well as multi-level analysis of selected teacher and student variables[2] provide the first ever research results that portray the common teaching practice of introductory electricity, its deficits and potentials for improvement.

Systematic, theory- and evidence-driven curriculum design – introductory optics

Although curriculum design has a long tradition in PER, it is often criticized for unclear or inconsistent methodologies as the theory-into-practice aspect frequently remains blurred.

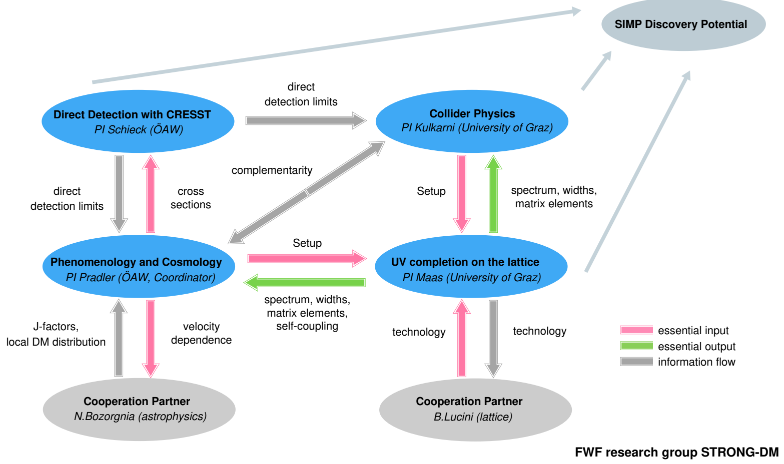


Design cycles and interventions in the design process of the optics curriculum.[3]

The DBR project on introductory optics[3] received special attention within the PER community as it reveales substantial insights in the systematic and rule-led process of curriculum development, its theoretical underpinnings as well as generated theories about teaching and learning introductory optics.

1 Schubatzky, T., Rosenberger, M., & Haagen-Schützenhöfer, C. (2019). Content structure and analogies in introductory electricity chapters of physics schoolbooks. Physics Education, 54(6), 065023
2 Schubatzky, T. (2020). Das Amalgam Anfangs-Elektrizitätslehreunterricht. Eine multiperspektivische Betrachtung in Deutschland und Österreich. (First PhD in Physics Education Research at the University of Graz)
3 Haagen-Schützenhöfer, C., & Hopf, M. (2020). Design-based research as a model for systematic curriculum development: The example of a curriculum for introductory optics. Physical Review Physics Education Research, 16(2), 020152.

Dark matter comes to Graz



The structure of the research group, depicting how information, technology, and results flow between the different subgroups, and with external partners.

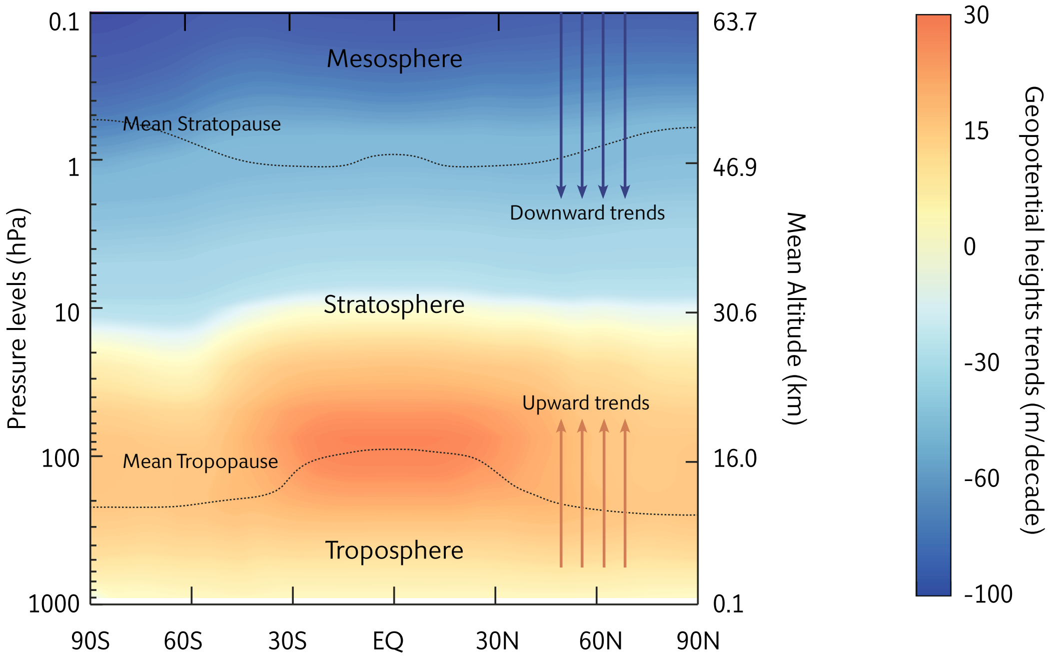
One of the most astonishing astronomical observations during the last hundred years is that the movement of stars inside our galaxies cannot be explained. The stars behave as if there would be almost five times as much matter as we see. Similar observations have been repeated over time for galaxies and even our universe itself. The simplest explanation for this would be the existence of a new form of matter. Because it does not emit light of any form, unlike ordinary matter, it has been dubbed dark matter. It is one of the biggest challenges in modern day particle physics and astrophysics - bound together in the field of astroparticle physics - to understand what dark matter is.

In 2020 the particle physics group in Graz, together with the ÖAW institute HEPHY, has joined this centennial effort. For this purpose it has won the first FWF research group at the University of Graz, and is only one out of three established in the first round in all of Austria. With about 8% success rate, this is an enormously competitive grant. Especially as this establishes a wholly new area of physics at Graz this underlines the excellent conditions for particle physics at the University.

The central pillar of this research group is a vertical integration through all relevant elements of dark matter physics: Experimental investigations covered by PI Schieck (HEPHY), astrophysical and cosmological constraints by PI Pradler (HEPHY), particle physics signatures at colliders like CERN by the newly established junior research group of PI Kulkarni (Graz), and the fundamental theoretical underpinnings by PI Maas (Graz). These activities at Graz are supported by further postdocs, PhD students, and master students. It is integrated into the doctoral academy of particle physics, and provides training in the field of astroparticle physics at both undergraduate and graduate level.

The genuinely unique research perspective is the combination of all relevant aspects, and its tight integration between theory and experiment. The aim will be to uncover whether it is possible that dark matter could actually be not a single particle, but rather a whole collection of new particles similar to the known quarks and gluons. If, they are expected to bind together, like quarks, to objects like a dark proton, which would then become the unknown dark matter. Ultimately, the research group will provide a complete workflow to understand how such dark matter behaves, and how it can be discovered. Using the most recent experimental and astronomical input will allow to decide, whether such strongly-interacting dark matter is feasible, or even confirm its existence.

Anthropogenic Contraction of the Stratosphere



Anthropogenic greenhouse gases change the structure of the atmosphere, © Petr Pisoft, Charles University, Prague.

One of the core research areas of the Atmosphere and Climate Physics Research Group is the study the Earth's atmosphere, employing novel satellite measurement techniques. In a recent work, developed through the collaboration of eight research centers in five countries, we could demonstrate, that the Earth's Stratosphere has contracted at a pace of more than 100 m per decade since 1980 and that the cause of this phenomenon is emissions of greenhouse gases. The results have been published in the renowned journal Environmental Research Letters:

Pisoft et al., Stratospheric contraction caused by increasing greenhouse gases, Environ. Res. Lett. 16, 064038 (2021).

While it is meanwhile common knowledge that the anthropogenic increase in greenhouse gases warms the Earth surface and the Troposphere, it is less known that increasing greenhouse gases cool the upper atmosphere, since (infrared) radiative cooling becomes more efficient. The Stratosphere, however, has also been cooling due to the decrease in stratospheric ozone (and thus reduced ultraviolet absorption). The warming of the Troposphere leads to its expansion, and therefore to an upward movement of its upper boundary – the Tropopause. Cooling of the Stratosphere, on the other hand, leads to a downward movement of its upper boundary – the Stratopause. We could show that the resulting contraction of the Stratosphere is primarily a consequence of increasing greenhouse gases – it will therefore continue, even after the recovery of the stratospheric ozone layer – as long as atmospheric greenhouse gas concentrations are increasing. Besides the fact that we are now even changing the structure of the atmosphere, this stratospheric contraction will serve as a very good indicator for anthropogenic changes in the atmosphere.

Overall structure and strategic setup

2. Overall structure and strategic setup

The research activities at the institute contribute to a wide range of challenges relevant to society, especially in the areas of energy, sustainability, environment, climate, digitalization and health. It does so in an interdisciplinary interaction with other institutes and faculties at the university, as well as in ubiquitous interactions with regional, national, and international partners.

One of the dominant contributors to all these areas will be nano and quantum physics. This topic forms the largest part of the research activities at the institute, carried by the research groups, „Surface Science" and „Theoretical solid state physics". These research groups have a very strong and documented collaborative approach, and form the primary research focus of the institute.

To cover the whole breadth of physics in teaching and research, this primary focus is complemented by a number of further research groups. The research group „Physics of atmosphere and climate" covers central questions of climate, environment, and sustainability. These areas are complemented by the research groups „Astro- and Solar Physics" and „Theoretical Particle Physics" working on fundamental questions about the nature of the universe, and the origin and properties of our solar system, and thus of us humans. Seeking answers to such questions is also an important element for raising the interest of the public in natural sciences as well as for recruiting new students. The research group „Didactics" is an indispensable part of the institute, as its research and development contributes to the improvement of physics education at schools and it guarantees well-educated new generations of physics teachers, who bring the essential skills and knowledge for a society build around science and technology in a suitable form to schools.

While not a research group in its own right, the topic of computational physics, at the very heart of any scientific digitalization pathway, is commonly carried by the research groups „Astro- and Solar Physics", „Physics of atmosphere and climate", „Theoretical Particle Physics", and „Theoretical solid state physics". This research area is not only one of the drivers of high performance computing at the University, both in terms of development and application, but also provides the necessary education to students in this rapidly developing and essential current and future field.

With respect to the GCP, it is mainly the primary research focus of nano and quantum materials, as well as computational physics, which will be enlarged by the research groups of the Technical University Graz. Strategically, it is therefore already now an important step that core research infrastructure, with lifetimes exceeding a decade, is created as common research infrastructure. Likewise intensive cooperations with groups from the TU Graz already pave the way to fill the idea behind the primary research focus of the GCP with life.

There are a number of primary individual research goals to be addressed by the involved groups in the coming years. The use of space-time structured light as a tool in a multitude of topics, ranging from biomedical applications to nano-material investigations, photonic active nano materials, and nano-structured material design. Within the field of nanooptics the development and understanding of plasmonic physics will be pushed to the realm of quantum effects, which will access novel phenomena. Given their prevalence, understanding the (nano) properties and structures of surfaces, especially their potential to interact in electric and chemical ways, is a major goal.

The development of tools and technology in these areas are both necessary steps as well as remarkable targets in their own right. Among these we list improved photonic devices, the use of optical forces, nanofabrication, quantum dots as tool to design light, magnetometry, and photoemission tomography.

In total, this will provide unprecedented insights into the features of matter and matter-light interactions at the nano-scale, including the interaction of different materials at surfaces. These will be decisive steps for the understanding and exploitation of nano and quantum materials.

Even though the other research groups do not have counter-parts at the TU Graz, cooperation at the center level is prepared by common interaction, especially in teaching, but also by involving TU Graz staff in hiring processes. Thus, in all search committees of these research group over the reported years members of TU Graz have been part. In addition, during the initial submission process for the Graz Center of Physics in 2018, the roles of these group in the GCP have been strategically put up together with the TU Graz, and will play the same role as they play for the Institute of Physics at the current time, representing the breadth of physics in teaching and research beyond the primary focus, despite being then much smaller in comparison to the full organization.

As a consequence, these foster strong cooperations with other research institutes, especially the Wegener Center at the University, and ÖAW institutes in Graz and Vienna. Especially, both the astrophysics group and the particle physics group push for structured research programs, like SFBs. Herein the group „Astro- and Solar Physics" focuses on the thriving field of stellar physics in the context of our own solar system and other stellar systems. The group "Theoretical particle physics" is strongly pushing to fully cooperate with the experimental activities in Austria, especially the involvement in CERN.

The group "Didactics" has its own, unique, profile by its very definition. Major goals are to research and develop strategies to improve digital competences of (future) physics teachers and their schoolstudents and to optimize strategies to transfer and implement innovative teaching concepts into active teaching practices. In this, they also drive new generations of students to start physics.

Within the common area of computational physics both the development of algorithms as well as the adaptation of modern technologies like GPU systems are important steps towards the future. A strong commitment to the usage of both local clusters as well as the VSC will provide continuous demand for upgrading these vital infrastructure. This plays well with the digitalization initiative of the University, and will be supported by more computational physics oriented appointments at all levels.

Within the next few years a number of professorships, at least two § 99.5 tenure track and three § 98 full professor positions, will be opened. Their individual foci will be discussed within the reports of the corresponding research groups. Filling these positions are decisive steps in implementing the strategic goals listed above. In addition, the institute has developed a long-range plan until when the GCP will take over the central role as a physics entity, for its development of personnel under the assumption of constant personnel budget. This common long-range plan documents the coherent strategic development process of the institute to have and maintain excellence in physics.

Research groups

3. Research groups

3.1 Research Groups with a focus on Quantum and Nano Materials

3.1.1 Nanoptics

Background

The Nanooptics Group investigates light on the subwavelength scale. Light is not only central to transmitting information spanning size scales from billions of lightyears to atomic dimensions, it also enables a wealth of applications in mobility, communication, medicine, sensors, data storage or material processing. In any case, diffraction limiting spatial resolution to about the wavelength, i.e. a few 100 nm is a major showstopper. An efficient approach to overcome this limit as pioneered by the Nanooptics Group is to apply plasmonic nanostructures to concentrate, manipulate and transport light on deep subwavelength scales. Enabling the work is an experimental toolbox involving nanolithography, near field microscopy, fluorescence and Raman spectroscopy, electron spectroscopy and time-resolved techniques, besides intense collaborations with theory groups. The Nanooptics research is structured in four fields and one associated group, as briefly described the following. Only key references since 2017 are listed.

Plasmonics with photons

Strong field enhancement and nanoscale light confinement make plasmonic nanostructures an intriguing research topic. We have recently looked into specific plasmon modes coupling weakly to light ("dark modes"), stacked nanoparticles and nanowires. Settling open questions with regard to the properties of regular nanoparticle arrays ("optical metasurfaces") that feature emerging phenomena as surface lattice resonances might contribute to their future application [1].

Plasmonics with electrons

While surface plasmons were first experimentally evidenced by electron energy loss spectroscopy (EELS), it was only recently that EELS, together with cathodoluminescence (CL) made its comeback in plasmonics. In cooperation with electron microscopy groups, we exploit the high spatial resolution of electron-microscopy-based EELS/CL, to analyze in detail surface, edge and particle plasmons [2]. On the other hand, photoelectrons emitted from metal nanoparticles that are accelerated in their fields prove valuable probes of plasmon near fields, as we investigate together with the Wigner Institute, Budapest [3].

Near field optics

We generate, image and apply optical near fields in tailored nanostructures. Besides scanning near field optical microscopy, we develop and use various plasmon field imaging schemes, as leakage microscopy, plasmon-based polymerization and plasmon-induced local heating [4]. We have found further attractive applications for plasmonic heating, e.g., to control thermoresponsive polymers.

Quantum dots and molecules

We investigate molecules and semiconducting nanocrystals (quantum dots) as photon single emitters [5] or emitter ensembles. For the latter, we looked into radiationless energy transfer, including the role of particle plasmons. Of fundamental as well as applied interest, we used the combination of plasmonic nanostructures and molecular layers to map plasmon fields and to control light extraction in organic LEDs [6]. Furthermore, we investigate photoconductance in closely packed quantum dot films.

Associated group Nanostructured Silicon – The Nanostructured Silicon Group applies nanostructured silicon as a matrix to fabricate ferromagnetic/semiconducting composites by chemical and electrochemical methods. The matrix formation allows the tuning of the pore diameters in a broad range from a few nanometers to several micrometers. The pores are filled with magnetic materials electrochemically or by chemical reduction to produce magnetic nanostructures with defined geometry. Our investigations mainly focus on the structural and magnetic properties of these hybrid materials, as the magnetic response strongly depends on their size, geometry and spacings. We pursue two main directions concerning the applicability in, first, magneto-electronics and, second, in biomedical drug delivery. With respect to the latter, we in particular examined the iron oxide nanoparticle size dependence in the context of magnetic interactions.

Highlights

Electron spectroscopy of plasmonic nanostructures with high spatial resolution

Reaching for nanoscale phenomena, bringing together fabrication, imaging and theoretical modelling at the smallest scales is key. About a decade ago, the Nanooptics Group initiated a close collaboration with the Centre for Electron Microscopy and Nanoanalysis at the TU Graz. Together with the theoretical developments of Ulrich Hohenester and his colleagues, EELS in high-resolution transmission electron microscopes was developed into a tool to yield signals closely related to those in optical measurements. With collaborations also extending to other international groups, EELS and in recent years also cathodoluminescence (CL) with nanometer resolution has by now significantly pushed forward our understanding of nanoscale optics. In recent work, we have shown by probing single nanoparticles that EELS and CL intensities correspond to extinction and scattering in optical spectroscopy, respectively, thus enabling to probe radiative and non-radiative components individually with nanometer resolution [2]. We have revealed that plasmonic cathodoluminescence faces a fundamental limit in spectral resolution due to the symmetry break induced by the trajectory of the probing electron beam itself [7]. Exploiting developments of the partner groups in 3D imaging and electron spectroscopy, we fabricated stacked nanoparticles with ultrasmall dielectric gaps that allowed to 3D image different coupled plasmon modes [8].

Spectrally tailoring, concentrating and enhancing light fields

With plasmonic nanostructures enabling the concentration of light of the deep subwavelength scale, we ask for the related ultimate limits. We use on one hand nanofabrication by electron beam lithography to geometrically tailor metal nanostructures, tailoring their plasmonic resonance frequencies and field profiles. We then combine nanostructures to form small gaps that sustain particularly strong local fields. Besides laterally coupled structures, the development of stacked nanodisks proved rewarding, as well-controlled isolating spacer layers just a few nanometers thick could be fabricated with high quality. Optical spectroscopy revealed the rich mode structure of these gaps [9], complemented by EELS characterization as discussed above [8]. As the smallest achievable gap size is however limited by the inherent roughness of lithographed surfaces, we also turned to chemically synthesized single-crystalline particles and gap-forming dimers thereof. In cooperation with the PREMS lab at the Paris Diderot University and the Center for Electron Microscopy at the McMaster University in Hamilton, Canada we investigated gold/silver nanocuboid dimers with atomically flat end faces and 3 nm gaps [10]. We complemented the experimental observation of strong coupling effects from this spectrally tunable geometry with simulated data, hinting at unprecedented high field enhancements in the gap.

Associated group Nanostructured Silicon

To enlarge the number of porous silicon template materials the Nanostructured Silicon Group started more than 10 years ago a close collaboration with the Department of Chemistry at the

Texas Christian University Fort Worth to implement silicon nanotubes for filling with magnetic nanostructures. On the one hand the novel systems are of interest for biomedical applications and on the other hand our research is associated with the fabrication of permanent nanomagnets by depositing bi-metal nanostructures with a softer and a harder magnetic phase [11]. In collaboration with GREMAN in Tours we investigate porous silicon with embedded magnetic nanostructures to improve the inductive behavior in on-chip RF devices. A further realm is the merging of optical and magnetic properties on one material level. In this regard a collaboration has been initiated with the Tokyo University of Agriculture and Technology and the University of Nagoya to investigate luminescent microporous silicon filled with magnetic materials with the purpose to enhance the photoluminescence efficiency. So far the dependence of the photoluminescence intensity, life time and spectral range on the metal loading could be shown [12].

Future developments

The agenda of the Nanooptics Group for the years to come is framed by the four research fields outlined in the Background section. Emphasis will however be shifted, as sketched in the following. Clearly, the existing optics and photonics focus of the institute (the experimental groups of P. Banzer and J. Krenn, theory cooperations with U. Hohenester) and novel opportunities related to the upcoming Graz Center of Physics are driving forces here.

First, preliminary work has been done or is underway for these topics, focused project stages are expected to follow in selected promising cases.

- **Plasmonic gaps.** Ever smaller and better controlled gaps generate not only improved field confinement, spectroscopic sensitivity or controlled hot electron generation, but approach as well the quantum regime with, e.g. electron tunneling taking place.

- **Plasmons and photoconductance.** Colloidal quantum dots in nanoscale metal gaps yield stable photocurrents, being thus a promising platform to investigate both, plasmon-controlled photoconduction processes and carrier photogeneration on the nanoscale.

- **Ultrafast transient spectroscopy.** In a cooperation with the group of Markus Koch, TU Graz we recently started ultrafast transient spectroscopy and microscopy on colloidal quantum dots. Femtosecond time resolution together with microscopy imaging is expected to open new information channels on the dynamics of complex hybrid nanostructures.

- **Strong field photoemission.** An established cooperation with the group of Peter Dombi, Wigner Institute, Budapest was recently extended by photoelectron electron microscopy in the group of Florian Lackner, TU Graz. We aim at understanding the dynamics of ultrafast strong field photoemission as well as applying it to measure, e.g., local field enhancement.

Second, these topics emerge from exploratory cooperations and could be taken up in due course.

- **Structured light** as pioneered by the group of Peter Banzer could significantly extend the range of optical characterization of plasmonic nanostructures.

- **Nanomanipulation** by a modified AFM (Banzer group) as a means to position individual nanoparticles could complement and extend established nanofabrication schemes.

- **Crystalline nanostructures.** Rather than with chemical synthesis, we look into ways of fabricating high-quality nanostructures by lithography on crystalline structures.

These exploratory perspectives build to a fair share on the continuity provided by existing experimental core equipment and its continuous upgrading. We note in this context that the actual technical personnel, maintenance and replacement conditions leave ample room for improvement.

- **Nanofabrication.** Fabrication of nanometer-sized metal, semiconductor or isolator structures with multi-step/layer fabrication options. The electron beam lithography system Raith eLine+, installed 2016 is a multi user NAWI Core Facility. Upgrades in the related thin film deposition systems.

- **Advanced force/near-field microscopy.** The Bruker/JPK Nanowizard atomic force microscope (AFM), installed 2020 enables 3-axis scanning of either the tip or the sample. It is combined with an optical microscope and spectrophotometer. Upgrades to conductive AFM.

- **Optical microscopy and spectroscopy.** Microscope setups are equipped with piezo-scanned stages, high-resolution spectroscopy and time-correlated single photon counting. Upgrades to confocal functionality and in laser sources.

Associated group Nanostructured silicon: The preliminary work concerning the enhancement of the photoluminescence of metal loaded porous silicon will be carried on and should aim at the exploitation of the metal plasmons to enhance the luminescence quantum efficiency and the findings of further magneto-plasmonic correlations. The newly started collaboration to fabricate on-chip RF devices with improved performance will be followed up. Furthermore, especially in the context of the mentioned topics we plan to investigate the electric properties of the hybrid materials and also include magnetic measurements at high temperatures (up to 950°C) to find phase transitions with respect to silicide formation.

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3.1.2 Optics of Nano and Quantum Materials (OPNAQ)

Background and Research Focus

The group Magnetometry and Photonics headed by Heinz Krenn for many years built up a very strong expertise in the fields of magnetometry, photoacoustic imaging/tomography as well as advanced spectroscopy, initiating intense collaborations with research partners and industry. In September 2020, Peter Banzer joined the faculty at the University of Graz together with part of his previous team from Germany. This date marks the inception of the new group Optics of Nano and Quantum Materials (OpNaQ) – Structured Light and Structured Matter. With the new team leader, the scientific portfolio of the group will now be extended substantially while also cultivating existing expertise and collaborations. With this step, two groups with complementary expertise, grown at separate places over decades, are brought together, aiming for the establishment of new research foci fostered by synergetic effects. Before joining the University of Graz, Peter Banzer was heading the research group Interference Microscopy, Polarization and Nano-Optics at the Max Planck Institute for the Science of Light (MPL; Erlangen, Germany) for more than 10 years. The pioneering experimental work and utilization as well as integration of light and matter engineered and interacting at nanoscale dimensions are at the heart of his former group. The research covered both fundamental and applied aspects of structured light and matter, introducing novel schemes and unique methods, uncovering intriguing optical phenomena and branching out to other communities such as integrated photonics, optical metrology, quantum optics, materials science, and optical communications. This knowledge, the corresponding versatile methods and techniques, part of the custom equipment as well as part of the former team were now transferred to the University of Graz to join forces with the groups at the Institute of Physics, and beyond. In addition, the existing national and international collaborations are further promoted, while actively seeking new collaborators strengthening the solid foundation for joint projects and grant proposals. Below, we briefly outline selected research activities of both (now unified) groups carried out during the reporting period.

Structured Light and Field Engineering

At nanoscale dimensions, confined light fields naturally feature complex and sophisticated distributions. We study collaboratively intriguing phenomena resulting from spatial confinement, explore novel applications, and develop versatile methods based on structured light-matter interactions, such as advanced spectroscopy, polarimetry and manipulation at the single particle level.

Novel Structured and Exotic Materials

With our methods, we study novel optical materials, which are either lithographically fabricated, self-assembled or nano-manipulated. Selected classes of quite unique materials are, e.g., novel carbon allotropes, metamaterials or materials featuring an electric permittivity close to zero. Several projects are based on joint efforts with international groups from St. Petersburg (Russia), Monterrey (Mexico), Erlangen (Germany) or Ottawa (Canada). These studies aim for the development of new materials with applications in manipulation and switching.

Novel Detectors, Integrated Photonics and Applications

We investigate how light can be coupled into and out of optical circuits efficiently using structured light. We study the efficient and controllable steering, mode-sorting and processing of light. We also co-develop a new integrated optical sensor platform, which will revolutionise the way we process light (H2020 FET-OPEN project SuperPixels). Furthermore, we explore applications of this detectors in nano-optics, communications, and imaging.

Nanometrology

We recently introduced a novel technique that allows for the experimental localization of single nanoparticles with sub-Angstrom precision. It is based on tightly focused vector beams for excitation and encoding the relative positon in a far-field distribution. With potential applications in microscopy and nanometrology, we currently work on the full integration of this scheme into a small-footprint device, offering also 3D and ultra-fast localization capabilities.

Photoacoustic Imaging, Tomography and Laser Ultrasonics

This research direction, mainly led by our experts Günther Paltauf and Robert Nuster, focuses on the development of generation, detection and image reconstruction methods for acoustic waves excited optically. In various collaborative projects with partners from other research centres and industry, we explore the capabilities of laser-generated sound in biomedical diagnostics and materials research.

Magnetometry and Solid State Spectroscopy

Our activities based on the profound expertise of Heinz Krenn, Peter Knoll and co-workers, focus on investigations of magnetic, superconducting and phononic properties of matter with focus on SQUID-magnetometry, FTIR- and Raman spectroscopy. The former Magnetometry and Photonics group has installed a widely used cryogenic infrastructure for non-standard tasks, which attracted the interest of external partners over the last two decades.

Quantum(-Inspired) Optical Experiments

Together with international experts from the quantum optics community (Erlangen, Glasgow, Ottawa), we also study the potential benefits of structured light or spatial field processing in quantum optics, e.g., for optical comm systems. Furthermore, we successfully adapted established schemes from quantum physics, such as weak-measurement-like protocols or correlations, for the study of nano and micro-systems.

Highlights

Magnetometry and Magneto-Optics

Improvement of magnetic properties (ultra-soft magnets) of metallic alloys by severe plastic deformation (at Erich Schmid Institute (ESI) of the ÖAW Leoben; ERC project). SQUID magnetometry combined with electrochemical deposition and potentiostatic measurements on lithium-ion batteries (FWF project P30070-N36, TU Graz).

Laser Ultrasonics

Laser-induced ultrasound for measuring properties of porous metal layers on or defects of silicon wafers (for semiconductor quality control).

Nanoscale Electromagnetic Field Phenomena and Measurements

First experimental demonstration of a direct measurement technique for electric and magnetic spin density distributions of confined light fields. Experimental demonstration and measurement of optical polarization structures in focal fields (topological light; international collaborations).

Development and Study of Novel Materials

Optical study of novel orthorhombic carbon flakes intercalated with metal particles, revealing an extraordinarily strong birefringence (international collaboration). First experimental study and demonstration of chiral surface lattice resonances.

Nanometrology

Experimental and theoretical demonstration of a novel sub-Angstrom and hi-speed localization method based on transverse Kerker scattering induced by structured illumination. Demonstration of an experimental scheme for precise dipole moment retrieval and maximised directional waveguide coupling (BMBF project 'HoChSeE'; with MPL).

Individual Nanostructure Spectroscopy and Phenomena

First demonstration of circularly polarized light emission from a linear dipole emitter. Proposal and experimental implementation of structured light enhanced Raman spectroscopy (international collaboration). First demonstration of the role of orbital angular momentum coupling in chiral light-matter interactions.

Quantum-Inspired Schemes and Methods

Proposal and experimental proof of weak measurement-inspired schemes based on structured light excitation/processing for enhanced metrology.

Future Prospects and Strategic Goals

The future activities of the newly established OpNaQ group will be based on the complementary expertise brought together by fusing two experienced groups. Collaborations with the experimental and theory groups at KFU and with external national/international partner will help in jointly bridging the gaps between several research communities, while laying the cornerstones for new directions. In this section, we compendiously showcase selected strategic goals.

Structured Light and Matter for Enhanced Photoacoustics and Laser Ultrasonics

Based on photoacoustic tomography (PAT) and microscopy (PAM) devices developed in recent projects, we will seek even closer collaborations with partners from biomedicine (e.g., via BioTechMed). In ongoing projects, we investigate the potential of photoacoustic imaging techniques for the quality assessment of organs before transplantation (FFG project). As a major research direction of the group, we plan to explore the great potential of nanostructured light and materials for implementing, testing and developing novel devices and techniques for the fields of PAM/PAT and laser ultrasonics (LUS). For instance, we plan to experimentally and theoretically survey the following novel concepts: 1.) sound wave detection based on artificially structured surfaces; 2.) bespoke light fields for enhancing contrast mechanisms and resolution; 3.) turbulence-mitigation-inspired spatial mode read-out for all-optical acoustic wave detection. In order to tackle these and other tasks, we plan to form strong national and international consortia to apply for corresponding funding. Some of the aforementioned tasks will be approached jointly with Joachim Krenn, Martin Lavery (Glasgow) and Robert W. Boyd (Ottawa).

Integrated Photonic Sensors, Detectors and Probes

We will focus on the development of camera prototypes based on SuperPixels, enabling spatially resolved measurements of light's intensity, polarization and phase. Also their application for the study of nano-systems at an unprecedented level of detail will play a pivotal role, with a special emphasis on nano-metrology and advanced microscopy. We also aim for the development of photonic all-integrated chip-based sensors for ultra-precise and fast motion tracking, nanoscale 3D polarimetry, and mode sorting. Several of the aforementioned goals will be tackled jointly with international partners, e.g., David Miller (Stanford), Sebastian Schulz (St. Andrews), and Alexander Bergmann (TU).

Optical Forces and Manipulation

We plan to investigate optical forces occurring when illuminating micron-sized particles with structured beams in a custom optical tweezers system. Focal field engineering leads to bespoke electromagnetic field landscapes providing for fine control over the forces acting on the particle. We plan to study exotic forces (Manuel Vesperinas, Madrid), new degrees of freedom for particle control, and photo-induced force microscopy (Israel De Leon, Monterrey).

Magnetometry, Optomagnonics and Magneto-Optics

The strong expertise and existing infrastructure in the field of magnetometry will act as a very fruitful ground for future activities, aiming mainly for the experimental study of magneto-optical or optomagnonic phenomena. Together with the group of Martin Sterrer, the liquid helium and SQUID infrastructure will be nourished and alternative routes will be explored to pave the way for future experiments. For instance, the purchased vibrating sample magnetometer will complement the SQUID-based infrastructure. Additional ideas centred on the coupling of light and magnons in magnonic crystals will be studied jointly with Silvia Viola-Kusminskiy (Erlangen) and Georg Schmidt (Halle).

Towards Extended Toolboxes for Advanced Nanoscale Spectroscopy and Polarimetry

We plan to extend our activities related to spectroscopy and polarimetry at microscopic and nanoscopic length scales, including the study of chiral, nonlinear or heterogeneous nanostructures and metasurfaces. Furthermore, we will intensify our activities as part of QuNET (BMBF), with our contribution centring on the study of custom optical fibres for quantum comm.

Quantum Sources, Matter and Phenomena

In a new research line, we will be dealing with the fabrication, experimental study and application of colour-centres in nanodiamond embedded in complex photonic environments. We are interested both in their quantum emitter and electronic spin state properties (with Christoph Becher (Saarbrücken) and Joachim Krenn). On the one hand, we aim for tailoring, manipulating and measuring the emission characteristics (BMBF project HoChSeE). On the other hand, we envisage the study of colour-centres for nanoscale magnetometry. At the same time, we will augment our customized setups optimized for structured light based experiments.

Development and Study of Novel Optical Materials

For several years now, we investigate optically a novel orthorhombic carbon allotrope intercalated with metal nanoparticles (collaboration Alina Manshina, St. Petersburg). Together we unveiled extraordinary optical properties. To fully understand the underlying crystalline carbon matrix and to explore applications, future steps will focus on a detailed optical and structural analysis, photon, electron and ion induced modifications, the application as integrated polarization elements, etc. In Graz, we team up with local partners (e.g., Roland Resel, TU; Martin Sterrer, KFU) to better understand the material system itself. In collaboration with the teams of Robert W. Boyd (Ottawa), we aim for the experimental investigation of another exotic materials, i.e., epsilon-near-zero materials, their interaction with structured light, and hybrid architectures, while polarization-dependent optical switches and nonlinear phenomena are in the focus. We will also intensify our studies of structured surfaces (Israel De Leon; Mexico; Thomas Weiss, KFU) with a focus on linear and nonlinear chiral effects.

Advanced Nanofabrication and Joint Infrastructure

In the context of customized optical setups, we want to make our technology also accessible to other groups, enabling synergy effects and laying the grounds for new project ideas. In a joint initiative with Gerald Kothleitner and Harald Plank at FELMI-ZFE as well as Joachim Krenn, we plan to build and implement an advanced nanomanipulation technique in Graz. The corresponding tool was originally developed in the former group in Erlangen. This system will enable the fabrication of complex nanophotonic hybrid systems.

Selected Publications

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3.1.3 Surface Science

Background

The Surface Science group is performing interdisciplinary research on surfaces, interfaces, and thin films. The interests of the group are in fundamental problems of nanoscience, ranging from organic electronics to catalysis. Our studies focus on the geometric, electronic, vibrational and chemical properties of atomically controlled surface structures (metals, oxides, molecular adsorbates) and are undertaken with a variety of surface science techniques, in ultrahigh vacuum, at ambient conditions and for solid-liquid interfaces. The research topics pursued in the group include five areas of both methodological and topical character, all related to nano and quantum materials and therefore encompass the main research directions of the GCP:

Photoemission tomography

The frontier orbitals of molecules are the prime determinants of their chemical, optical and electronic properties. The most direct method of addressing the (filled) frontier orbitals is UPS and our work has shown that the UPS angular distribution can be simply understood and considered to give an image of the orbitals in reciprocal space. This has opened up a new experimental window for the study of molecular adsorbates and films.

Molecular thin films and their interfaces

Functional organic molecules and organic semiconductors, and their interfaces with both inorganic and organic substrates, are relevant in modern technology. We investigate the morphological, electronic, and chemical properties of organic molecules and their specific interaction at interfaces from the single-molecule level to monolayers and thin films.

Ultrathin oxide films

Due to the ubiquity of oxygen in the environment, many real surfaces are covered by a thin layer of oxide. Our work aims at the controlled fabrication of well-defined ultrathin oxide films and nanostructures on metal surfaces. The thickness confinement and presence of the metal substrate can result in the stabilization of novel phases of the materials and lead to unexpected physical and chemical properties.

Model catalysis

Oxides and oxide-supported metal nanoparticles represent important classes of materials in heterogeneous catalysis. We prepare single-crystalline oxide thin films and metal nanoparticles thereon as models of real catalysts. Among the various aspects of catalysis, we specifically focus on the elucidation of metal-support interactions, reactivity of oxide surfaces, and model approaches for catalyst preparation.

Solid-liquid interfaces

Solid-liquid interfaces play an important role in both technology (energy, corrosion, electrocatalysis) and environment (weathering, soil chemistry). Extending surface science approaches to solid-liquid interfaces represents a challenge. With in-situ studies of interfaces between well-defined surfaces and aqueous electrolytes we aim to gain fundamental, atomic-scale understanding of the structure, adsorption behavior and electrocatalysis at solid-liquid interfaces. Overall, the aims of our studies are to create well-defined model surfaces/interfaces in ultrahigh vacuum and understand, control and tune the morphological and electronic properties of the materials at the atomic/molecular scale. This allows the correlation of surface structure to properties (e.g. reactivity) and gain fundamental insights into surface/interface processes.

For this purpose, we presently run 11 ultrahigh vacuum machines equipped with tools for preparation and in-depth characterization of surface structures, including photoemission spectroscopies (angular-resolved UPS, XPS), scanning probe microscopies (STM, AFM) and vibrational spectroscopies (IRAS, HREELS). In addition, specific set-ups for in-situ studies of solid-liquid interfaces (cyclic voltammetry, electrochemical STM, and vibrational sum frequency generation spectroscopy) are in operation. In the reporting period we could expand our experimental toolbox with the help of significant financial support from in-house infrastructure initiatives and regional infrastructure funds. These included the installation of a preparation and characterization chamber at the NAWI Graz core facility NanoPEEM, the installation of a new cryo-STM/AFM, and the electronics upgrade of a VT-STM.

The interdisciplinarity of the groups research is reflected in several local, national and international collaborations:

Uni Graz: Solid-state theory group (Puschnig); Physical and theoretical chemistry (Grill, Boese)

TU Graz: Institute of Experimental Physics (Schultze), Institute of Computational Physics (von der Linden), Institute for Chemistry and Technology of Materials (Gollas, Abbas)

National and international: JKU Linz, (Stadler); LFU Innsbruck AT (Bertel); FZ Jülich, DE (Tauz); PTB Berlin, DE (); HZB Berlin, DE (Rienks); FHI Berlin, DE (Freund); HU Berlin, DE (Paier); Univ. Tübingen, DE (Chassé), UN Cordoba, ARG (Negreiros); University of Nova Gorica, SLO.

Highlights

Photoemission tomography and molecular thin films and interfaces

We have been establishing the foundations of photoemission tomography as a quantitative technique for studying both electronic and geometric structure. This has involved investigations of numerous molecules on both metals and dielectric thin films both in the home labs and at the PTB´s synchrotron. The orbital-by-orbital characterization of molecular monolayers by PT has yielded molecular orientation, orbital energy ordering and degree of charge transfer at the interface.[1] In doing so it has also provided important benchmarks for developing ab initio electronic structure calculations. A particular highlight was using PT to identify on-surface reaction pathways and products.[2]

Charge transfer across interfaces

By a combination of LT-STM and PT studies, we could demonstrate that introducing thin insulating layers between a metal substrate and a molecular adsorbate can increase the amount of charge transferred to the molecule. Not only could we quantify charge transfer to molecules, but we could also distinguish between, and quantify, charged and uncharged species on the dielectric films, which resolves some confusion regarding the electronic level alignment of, and charge transfer to, organic films on dielectric interlayers. In our atomically controlled study we demonstrated that the relationships of the controlling parameters are very simple and express the pure physics at dielectric interfaces.[3]

Ultrathin oxide films

We fabricated, using molecular beam epitaxy techniques, a crystalline 2D WO_3 overlayer on a Ag(100) surface and unveiled its geometric, electronic, and vibrational structure. The 2D WO_3 phase forms a bilayer with a staggered arrangement of WO_6 octahedra, linked together by corner- and edge-sharing, which is significantly different from the cubic and monoclinic WO_3 bulk structures, but resembles a bilayer of the α-MoO_3 layered bulk lattice. Such a 2D WO_3 bilayer on Ag(100) is a robust nonpolar structure, which is weakly coupled to the metal substrate, and should survive as a stable freestanding layer, that is, as a nanosheet.[4] In the past two years we have extended this topic to the fabrication of MoO_3 and WO_3 ultrathin layers on Pd(100) surfaces, which form the basis for the preparation of tungsten and molybdenum bronzes by doping and reaction with alkali metals.

Model catalysis and solid-liquid interfaces

In this research area we have been following three main research topics. On the one hand, the interaction of metal and oxide surfaces with a variety of molecules has been investigated. To mention here are the first imaging of the ordered water monolayer on MgO(001), and the bonding and thermal stability of cysteine, an amino acid, and catechol on Pt and iron oxide surfaces.[5-7] On the other hand, we have been interested in adsorption-induced roughening of metal surfaces and investigated specifically the influence of cyanide groups on the morphology of Pt(111) and Au(111) surfaces and Au nanoparticles in solution environment.[8,9] Finally, we have successfully extended our model approach to catalyst preparation to Au nanoparticles on ceria surfaces and could demonstrate the influence of chloride ions on the dispersion of Au nanoparticles.

Future developments

New §99.5 professorship in Surface Science

By the beginning of 2022, a new §99.5 professorship (tenure track) in Surface Science will be installed. The new colleague will strengthen and support the Surface Science group in one of the research areas introduced above.

Extending photoemission tomography into the ultrashort time domain

Extending photoemission tomography into the ultrashort time domain will provide novel fundamental insights, e.g. by investigating dynamic processes in solid state physics (excitons) or by following electronic processes occurring during chemical reactions directly. In collaboration with Martin Schultze (TU Graz) first time-resolved experiments at the NAWI Graz core facility NanoPEEM are planned. In addition, within the FWF Joint International Project "Photoemission Tomography of Excited Molecular States", a cooperation between the quantum optics and ultrafast XUV laser physics group at the University of Nova Gorica (Slowenia), the ab-initio electronic structure theory group and us has been started. The aim of this project is to use photoemission tomography (PT) to elucidate the formation, diffusion and decay processes of excited molecular states (excitons) in organic semiconductors

Establishing the fundamentals of charge transfer through and at dielectric films

With our previous work we have set the basis for an in-depth understanding of charge transfer processes through ultrathin dielectric films. In the years to come, we plan to expand this topic to more complex systems, including molecules, which feature functional groups that form covalent bonds with surfaces. In addition, we plan to address the local influence of charged surface defects on dielectric surfaces on charge transfer into molecules and elucidate the chemical reactivity of charged surface structures (metal atoms vs. organic molecules).

Self-metalation reactions of porphyrins on oxide surfaces

Porphyrins are among the most important naturally occurring macrocycles. Their interaction with metal surfaces has been extensively studied in the past. However, relatively little is known about the interaction with oxides. In particular, the mechanism of the self-metalation reaction remains elusive. Our initial studies on the adsorption of porphyrin molecules on ultrathin oxide films provide evidence for the interplay of charge transfer into and substitution of the macrocycle on the self-metalation activity. Our future studies of porphyrin adsorption and assembly on, both, metal and oxide surfaces aim at the elucidation of self-metalation and chemical reactivity of porphyrins at interfaces.

Creating a scientific basis of 2D oxides for energy applications

The project's ultimate goal is to investigate the doping of atomically-thin 2D WO3 and MoO3 metal-supported model systems with alkali atoms and elucidate the modification of their structural, electronic and vibrational properties at the atomic level by a combination of state-of-the-art experimental and theoretical methods. Detailed understanding of the doping behaviour of 2D oxide layers will allow to establish the scientific basis for the design of AxWO3 and AxMoO3 oxide nanostructures with a potential use in future energy-related applications.

Model catalysis with single site catalysts

We plan to expand our studies on model catalysts to specific single-site systems. In collaboration with Nadia Mösch-Zanetti (Institute of Chemistry, Uni Graz), we will prepare bio-inspired, supported single-site metal centers on surfaces to elucidate the mechanism of specific catalytic reactions.

Electrochemistry of oxide-supported metal nanostructures

Initial ex-situ studies performed in the last year have provided first insights into the stability and surface roughening of metal single crystal surfaces and oxide-supported metal nanoparticles, and the corresponding reactivity, in electrochemical environment. In future studies we plan to explore adsorption and electrochemical-induced, structure-sensitive morphological changes at solid-liquid interfaces in more depth using in-situ techniques and establish model surface science studies of electrochemical and electrocatalytic processes.

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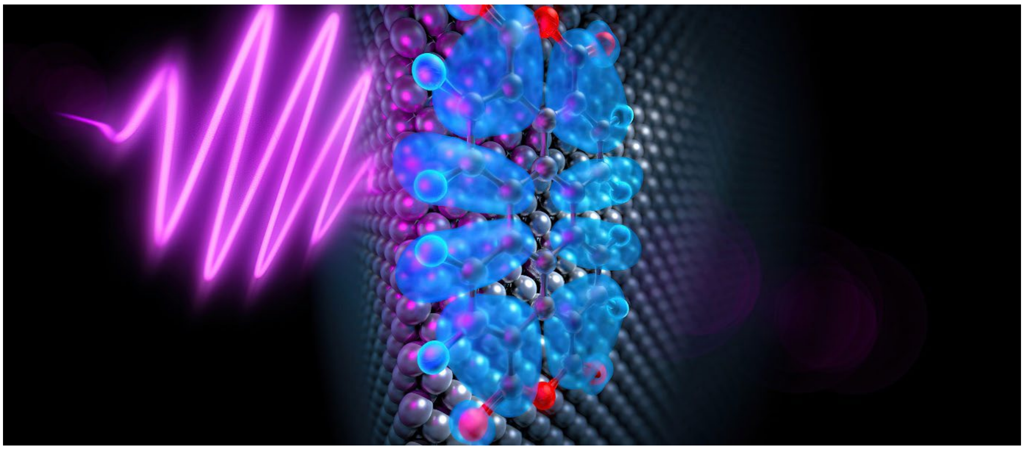
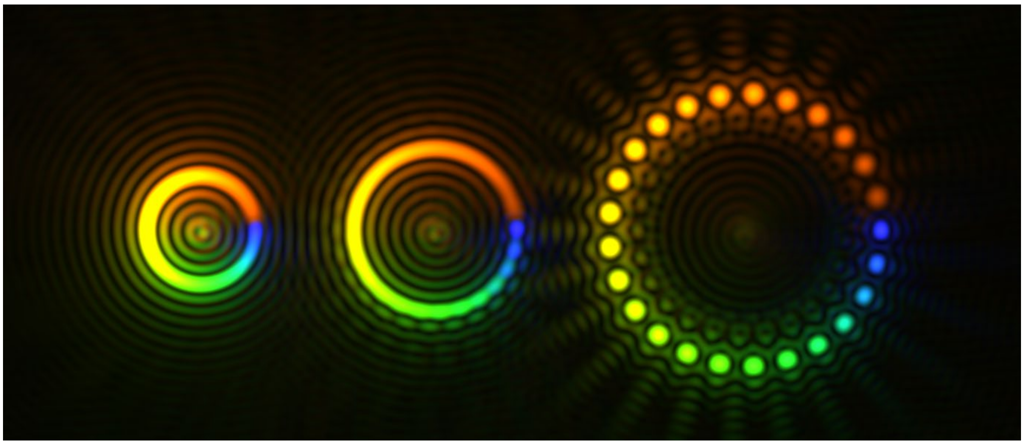
3.1.4 Theoretical Solid State Physics



Photoemission tomography by Peter Puschnig, © Till Schürmann, Philipps-Universität Marburg



Nano optics simulation, © Ulrich Hohenester

State of the art

Solid-state theory is a discipline of physics dedicated to establishing a fundamental quantitative understanding of the physical properties of solid matter, the prediction of new phenomena, and the evaluation of their potential for technological application. As such it has far-reaching impact on both other areas of physics and technological progress in our society. The contribution of the theoretical solid-state physics group at the University of Graz focuses on the area of nanophysics, a field which in the last few decades has provided some of the major hot topics in physics and innovative technology alike. Modern computers have made possible the atomistic simulation of complex nanostructures which in turn provide a direct comparison with and/or interpretation of experimental results, as well as guidance for future experiments.

The current research portfolio of the three permanent members includes topological solid-state physics (Walter Pötz), density functional theory (Peter Puschnig), and nano optics and plasmonics (Ulrich Hohenester). Focal research efforts of the current solid-state theory group include: quantum transport and spintronics; ab-initio density functional theory calculations of electronic and optical properties in the field of surface physics; simulation of light-matter interaction and plasmonics at the nanoscale. The theoretical solid-state physics group is engaged in analytic and numerical model development and simulations. As such it is a core discipline of Quantum Matter – a key theme of the to be formed Graz Center of Physics, the Computational Physics theme of the Department, as well as the Nanoscience effort of the University of Graz.

In the past the solid-state theory group has successfully collaborated with several experimental groups in house and at the TU Graz, including the surface science, nano optics, and electron microscopy groups. Numerous joint publications in internationally renowned journals have emerged from these collaborations. As a team player, the solid-state theory group is well embedded in the environment of the Graz Center of Physics and plans to play a collaborative role in its formation process.

Strategy for the coming years

The main change of the solid-state theory group in the coming years is the start of Thomas Weiss on August 1st 2021 as a successor of Walter Pötz. He is an expert in numerical and semi-analytical methods in linear and nonlinear nanophotonics. He has successfully collaborated with many international groups and will continue these collaborations when joining the University of Graz. There are ongoing projects at the University of Stuttgart with Na Liu on active plasmonics using DNA origami and Harald Giessen on structural colors using silicon nanophotonics. He will also continue his collaborations with Markus Schmidt (University of Jena) on nonlinear properties of leaky modes in optical fibers. On the theory side, he will work together with Egor Muljarov (Cardiff University) and Nikolay Gippius (Skoltech) on the theory of resonant states and advanced numerical methods.

In Graz, Thomas Weiss plans to establish close collaborations with Peter Banzer on chiral nanophotonics as well as the nonlinear properties of epsilon-near-zero materials. Furthermore, joint projects are envisioned with Joachim Krenn on nanophotonic sensing and imaging. Regarding chiral and achiral sensing of single and few molecules in the vicinity of nanoresonators, Thomas Weiss will benefit from the expertise of Daniel Boese at the University of Graz as well as the groups of Hofmann, Bergmann, and Schultze-Bernhardt at the TU. Finally, Thomas Weiss will also collaborate with Ulrich Hohenester on the resonant interaction of nanoantennas in ordered and disordered configurations.

Peter Puschnig plans to employ a time-dependent density functional approach to study time-resolved photoemission tomography (collaboration with Prof. Rubio, MPI Hamburg), and with a renewed focus on the ab-initio description of optical excitations via many-body perturbation theory, the theoretical framework for understanding the ultra-fast excitation dynamics of nanostructures at surfaces will be provided.

This will foster future collaborations with the surface science group of Martin Sterrer and the laser physics group of Martin Schultze (TU Graz) using their joint research core facility "NanoESca Lab" which will allow state-of-the-art pump-probe photoemisson tomography experiments.

Ulrich Hohenester plans to continue the successful collaborations with the nano optics group and the electron microscopy group. Currently he establishes a collaboration with the group of Christian Hill at the Medical University of Graz on optofluidic force induction, which includes the supervision of a joint PhD student. Also, a collaboration with the Group of Peter Banzer is foreseen.

Highlights

With two Science papers in early 2021 the solid-state group has recently underlined its superb quality of research.

The research highlights of Walter Pötz include the development of (the first truly) single-cone finite-difference schemes in 2d and 3d space dimensions; a generalized formulation of perfectly matched layer boundary conditions, and their application in Dirac fermion simulations.

The research of Peter Puschnig has recently been focused on the development and application of photoemission tomography, a technique which has been coined in Graz through the collaboration of the surface science group. This has led to a number of high-impact publications including papers in Science (2021), Nature Communications (2019), Angewandte Chemie (2020) or ACS Nano (2020), and to the development of a toolbox for simulation and experimental data analysis in photoemisson tomography (Comp. Phys. Commun., 2021).

Through a collaboration with experimental groups from the Forschungszentrum Jülich and the University of Marburg, the most recent highlight "Tracing orbital images on ultrafast time scales" in Science 371, 1056 (2021), demonstrates how photoemission tomography can be extended to study to the time domain. By combining tomographic photoemission imaging with a femtosecond pump-probe scheme, the excited state molecular orbitals of surface-adsorbed molecules can be traced in time thereby opening a new window for investigating the ultrafast electron transfer dynamics in such processes as chemical reactions on surfaces and intermolecular charge transfers.

The research highlights of Ulrich Hohenester include a paper in Science (2021) and a textbook published with Springer (2020). In collaboration with groups at Orsay and the TU Graz, a paper on "Three dimensional vectorial imaging of surface phonon polaritons" has been published in Science 371, 1364 (2021). It reports the first three-dimensional imaging of infrared-fields of surface phonons in a MgO cube using electron microscopy. The contribution of the solid-state group has been the development of a novel 3D-reconstruction scheme for electromagnetic fields, as well as the tomographic reconstruction of these fields using the experimental EELS data as input. The textbook "Nano and Quantum Optics" by Ulrich Hohenester is a modern primer on the rapidly developing field of quantum nano optics which investigates the optical properties of nanosized materials. The essentials of both classical and quantum optics are presented before embarking through a stimulating selection of further topics, such as various plasmonic phenomena, thermal effects, open quantum systems, and photon noise.

3.2 Complementary Research Groups

3.2.1 Astro- and Solar Physics

Current Status

The research group Astro- and Solar Physics has two main research foci: (a) the physics of the Sun and the heliosphere, and (b) the physics of stars and their environment.

The research topics of the solar and heliospheric group cover the dynamics of the solar photosphere, the physics of solar flares, coronal mass ejections (CMEs), solar wind as well as the interaction processes and space-weather impact at Earth and other planets. The group is strongly driven by an observational approach, and over the last decade became a world-leading group on the diagnostics and physics of solar eruptions and CME propagation in interplanetary space. In recent years, also a branch on modeling of the coronal magnetic field and MHD processes was established, through subsequent successful third party projects (primarily through scientists acquiring their projects as "Selbstantragsteller"), which provides an important complement for the studies of solar eruptions. The stellar research focus is on stellar activity and studying the structural evolution of solar analogues through asteroseismology of solar-like oscillating stars, stellar activity indicators, and theoretical stellar modeling. Studying stars like the Sun provides the opportunity to learn about our host star's past, present, and future and their potential as hosts of exoplanets.

The solar and stellar research teams benefit from their interactions and the in-house interdisciplinarity in state-of-the-art topics. The exchange in the fields of solar and stellar activity has become a highly important topic, in particular due to its relevance for the characterization and habitability of extrasolar planetary systems. These synergies were systematically developed and strengthened over the last decade, and place the group internationally into a strong position. This complementary solar-stellar research approach shall be further strengthened with the §98 Professorship (NF Hanslmeier) to be filled in the upcoming years in the field of stellar astrophysics.

The Astro- and Solar physics group regularly publishes a high number of well-cited papers in the important Journals in the field as well as high-impact Journals. The group has and is continuously performing a substantial number of third party research projects acquired in competitive processes at national as well as international level (main funding agencies: FWF, FFG, ESA, EU). These projects are led by staff but also by a considerable number of successful self-applicants. This is a strength, as it demonstrates the high international standing and competitiveness of the group. But it also is a vulnerability, as there is a subcritical fraction of staff to third-party researchers which endangers continuity. This is now getting pressingly relevant with the new UOG that limits the employment contracts of third-party funded researchers.

Research Infrastructure

The group runs two observatories: Kanzelhöhe Observatory for Solar and Environmental Research[1] (KSO) and Observatory Lustbühel Graz (OLG). KSO is mainly for research purposes. It performs high-cadence full-disk observations of the Sun in white-light, H-alpha and Ca II K as well as automatic detections of solar flares and filaments. The data are all fully searchable and available to the community on our data servers. They are used for research by scientists all over the world, sent to the World Data Center (WDC) for sunspot recordings, and contribute to ESA's Space Safety Space Weather program. OLG is for teaching and research purposes, mostly for studies on stellar activity and follow-up observations for exoplanet candidate detections from the NASA TESS space telescope. OLG is also a station of the international e-CALLISTO radio spectrometer network.

1 Note that KSO has also a focus on environmental science. This part connects to the Atmosphere and Climate Research Group and is not described here.

The group works also with data from a large number of current ESA and NASA space missions as well as the high-resolution ground-based telescopes on the Canarian islands and the European Southern Observatory (ESO). The group is a Co-I organization and co-developer of the Spectrometer Telescope for imaging X-rays (STIX) onboard Solar Orbiter (launched in February 2020), which is currently ESA's most important solar and heliospheric space mission. The group is also involved in the European Solar Telescope (EST) initiative, driven by two H2020 projects.

Highlights

The group has provided the first comprehensive characterizations of coronal dimmings, a signature of magnetic field "opening" and mass loss associated with coronal mass ejections (CMEs). These include determination of dimming parameters, their relation to flares and CMEs (Dissauer+ 2018a,b,2019, Chikunova+ 2020), plasma characteristics and flows (Vanninathan+ 2018, Veronig+ 2019), as well as their relation to the magnetic topology and initiation of CMEs (Prasad+ 2020).

Systematic studies on occurrence rates and detection of CMEs on late-type stars were carried out, which have important implications for stellar evolution and the habitability of exoplanets (Vida+2019, Odert+ 2020a,b, Leitzinger+ 2020, Koller+ 2021). The first benchmarking of dimmings as CME indicator was performed using Sun-as-star EUV measurements, and a new method for stellar CME detection was established. 21 CME candidates were identified in stellar EUV and X-ray light curves, which is more than all previous stellar CME reports (Veronig+ 2021, Nat. Astr.)

Observational methods and modeling approaches based on magnetic helicity were developed in order to obtain a better understanding of the energy release process and the eruptivity of solar flares (Tschernitz+ 2018, Hinterreiter+ 2018, Veronig+ 2018, Thalmann+ 2019, 2020) and to provide automatic flare detections (Pötzi et al. 2018). A particular relevant finding is the magnetic confinement, i.e. the suppression of flare-associated CMEs originating in strong Active Regions (Li+ 2020), due to their implications for the solar-stellar scalings of CME occurrence.

Comprehensive studies were performed on solar coronal holes, their magnetic characteristics (Heinemann+ 2018b, Hofmeister+ 2019), plasma properties (Saqri+ 2020, Heinemann+ 2021), and their relation to high-speed solar wind streams at Earth (Temmer+ 2018, Heinemann+ 2018a, Hofmeister+ 2018, 2020) and Mars (Geyer+ 2021). Ensemble CME propagation models (Dumbovic+ 2018) and a novel approach deriving CME volumes and mass exchange between CME magnetic/sheath structure and solar wind was developed (Temmer+ 2021).

In addition, new Deep Learning methods have been developed in order to provide quality assessment, enhancement, long-term homogenization and segmentation of solar imaging observations (Jarolim+ 2020, 2021).

Exploitation of the asteroseismic data acquired by NASA's Kepler and TESS missions resulted in studies on the evolution of internal stellar rotation (Tayar+ 2019), age dating of events in the galactic history (Chaplin+ 2020), and sample studies with up to 30000 solar-like oscillators in advanced evolutionary phases (Mackereth+ 2021). Group-members are also involved in the work-package preparation for the forthcoming ESA Plato mission (launch foreseen in 2026). Combining the Austrian BRITE satellites with the high-resolution SONG spectrograph, Beck+ (2020) has obtained the first spectro-photometric time series of bright red giants which opens the path to measure the level of adiabicity in evolved stars.

Research awards to young scientists of the group

Dr. Karin Dissauer: Josef Krainer Förderungspreis 2020 für PhD thesis

Dr. Stefan Hofmeister: PhD Thesis Prize 2020 of the Solar Physics Division of the European Physical Society EPS as well as the "Award of Excellence 2020 des Bundesministers für Bildung, Wissenschaft und Forschung" for PhD thesis.

Robert Jarolim, MSc: Early-Career Award (Best Poster) at international conference on Machine Learning in Heliophysics, Amsterdam, 2019 as well as the "Würdigungspreis des bmbwf für die besten AbsolventInnen von Diplom- bzw. Masterstudien" 2020/21.

Publications in high-impact journals

Mattila, S. et al. (2018): A dust-enshrouded tidal disruption event with a resolved radio jet in a galaxy merger, Science 361, 6401, 482-485. *https://doi.org/10.1126/science.aao4669*

Grant, S.D.T., D.B. Jess, T.V. Zaqarashvili, et al (2018): Alfven wave dissipation in the solar chromosphere, Nature Physics 14, 5, 480. *https://doi.org/10.1038/s41567-018-0058-3*

Samanta, T. et al. (2019): Generation of solar spicules and subsequent atmospheric heating, Science 366, 890. *https://doi.org/10.1126/science.aaw2796*

Gou, T., R. Liu, B. Kliem, Y. Wang, A. M. Veronig (2019): The birth of a coronal mass ejection, Science Advances 5, 10. *https://doi.org/10.1126/sciadv.aau7004*

Srivastava, A. K. et al. (2018): Confined pseudo-shocks as an energy source for the active solar corona, Nature Astronomy 2, 951-956. *https://doi.org/10.1038/s41550-018-0590-1*

Chaplin, W.J. et al. (2020): Age dating of an early Milky Way merger via asteroseismology of the naked-eye star ν Indi, Nature Astronomy 4, 382. *https://doi.org/10.1038/s41550-019-0975-9*

Temmer, M. (2021): Space weather: the solar perspective, Living Reviews in Solar Physics, Volume 18, Issue 1, article id.4, *https://doi.org/10.1007/s41116-021-00030-3*

Veronig, A.M, P. Odert, M. Leitzinger, K. Dissauer, N.C. Fleck, H.S. Hudson (2021), Indications of stellar coronal mass ejections through coronal dimmings, Nature Astronomy 5, 697-706. *https://doi.org/10.1038/s41550-021-01345-9*

Strategic Aims

An important development in the upcoming 3-year period will be the opening of the §98 Professorship (NF Hanslmeier). This professorship shall be announced in the field of stellar astrophysics, including topics like stellar activity, stellar evolution and exoplanets. Strategically, this professorship shall be another corner stone with respect to the §99.4 Professorship Solar Physics (Veronig) and the research groups at the Institute of Space Research (IWF) of the ÖAW in Graz (space plasma physics, planetary atmospheres, exoplanets, space-based instrumentation), in order to have complementary but close-enough research fields that allow bilateral and multi-lateral interactions and collaborations between different subfields and groups in Graz. This strategy shall also enable us to finally gain critical mass and the necessary minimum number of PIs to lead FWF SFB or DK initiatives. This strategic development is also placed in the framework of the GCP, where new positions and stronger interconnections with IWF and TU Graz in the field of stellar astrophysics were foreseen. With the inauguration in October 2021 of Prof. Christiane Helling as new Director of the IWF and Professor at the TU Graz, this strategy is indeed excellently placed as Prof. Helling is an astrophysicist with main research focus on exoplanets.

The current research topics on various aspects of solar and stellar activity will be further developed. The solar research in the upcoming years will be shaped by the ground-breaking ESA/NASA Solar Orbiter Mission (where the group is Co-I on the STIX instrument), which will enter its science phase.

Further participation in new space missions has recently be selected by NASA (SunCET - The Sun Coronal Ejection Tracker Concept; cube-sat mission with an extreme ultraviolet imager and spectrograph instrument). Current stellar astrophysics and exoplanet research are based on the ongoing NASA TESS mission, unprecedented in photometric quality, and the number of target data. In 2026, ESA will launch the next generation photometric space telescope PLATO to continue asteroseismic and exoplanet research. An FWF SFB concept proposal led by the Institute of Astrophysics of the University of Vienna was recently selected for full-proposal stage. This SFB envisions to study the evolution of Earth, Venus and Mars, to advance our understanding of how the atmospheres and surfaces of these planets evolved to their current states and why all three followed completely different evolutionary pathways. This interdisciplinary approach brings together researchers in geosciences, atmospheric sciences, and astrophysics.

An important aspect to be addressed in the upcoming years is the recently established new UGO that limits the employment of third-party funded researchers, even in cases where they bring in their own money. This new law strongly affects the Astro- and Solar Physics Research Group, which was successfully developed into a strong group over the last decade, despite the very limited number of permanent scientific positions. This means that new structures at the university/institute need to be discussed and created, like for instance, unlimited term contracts for third-party funded scientists, university-funded positions offered to excellent scientists that were successful in their third-party projects for extended periods, etc.

3.2.2 Atmosphere and Climate Physics

Current Status

Research in this area is performed in close cooperation with the *Atmospheric Remote Sensing and Climate System* (ARSCliSys) Research Group at the *Wegener Center for Climate and Global Change* of the University of Graz. Even though ARSCliSys is primarily located at the Wegener Center (and therefore within the URBI Faculty), 15 % of its acquired funds and research output are allocated to the Institute of Physics. At professor level, the joint group currently consists of Assoc. Prof. Ulrich Foelsche (Institute of Physics), and Prof. Gottfried Kirchengast as well as Prof. Andrea K. Steiner (Wegener Center). Research of the group contributes significantly to the Field of Excellence Climate Change Graz at the University of Graz. UF, GK, and AS are faculty members of the FWF-funded DK (Doctoral Programme) Climate Change.

The Atmosphere and Climate Physics group is very successful in acquiring third party funding (FWF, FFG, ESA) and publishes regularly in the leading journals in the field. Acknowledging that such evaluations are not always representative, it is still worth mentioning that "Atmospheric Science" was the highest-ranked subject at the University of Graz in the 2021 *Shanghai Ranking*: https://www.shanghairanking.com/institution/university-of-graz

Main research topics (RTs) are

RT (1) GNSS radio occultation for climate monitoring, diagnostics, and processes

The group is among the pioneers and world leaders in the field of atmospheric remote sensing that employs radio signals from GNSS (Global Navigation Satellite System) satellites in occultation geometry for atmospheric and climate science and applications. The GNSS radio occultation (RO) technique is meanwhile established as one of the most important observing methods for numerical weather prediction and satellite-based global climate monitoring. The international standing of the research group is reflected by the fact that UF is one of the two co-chairs of the *International Radio Occultation Working Group* (IROWG), a permanent working group of the *Coordination Group for*

Meteorological Satellites (CGMS); AS is co-chair of the Activity *Atmospheric Temperature Changes and their Drivers* (ATC) of the *World Climate Research Programme* (WCRP); and GK is permanent member of the Radio Occultation Science Advisory Group (RO SAG) of the European Space Agency (ESA) and the European Meteorological Satellites Organization EUMETSAT. The main aim of this RT is to establish benchmark-quality RO records of essential climate variables of the atmosphere, such as temperature and water vapor, and to use them for high-level climate diagnostics and processes studies.

RT (2) Climate and hydrology change monitoring and analysis at regional-local scale

The main aim of this RT is to perform frontier research on climate-hydrology change to understand processes that govern regional and local variability and changes in the European Alpine region, with focus on analyzing hydrological extremes (heavy precipitation, droughts) in a warming climate. This is done by exploiting the unique WegenerNet station network with 1-km scale resolution for studies such as evaluating convection-permitting climate models, validating satellite and ground radar data, and exploring properties of heavy precipitation at very high resolution.

The WegenerNet is very well suited for the validation of satellite data, like those from the NASA *Global Precipitation Measurement* (GPM) mission. UF is member of the NASA PMM (Precipitation Measurement Missions) science team and Principal Investigator (PI) of the project *Direct validation of GPM products with data from the high-resolution WegenerNet meteorological station networks in Austria*. In 2020, the *European Space Agency* ESA selected the WegenerNet as validation site for the upcoming Earth Explorer satellite mission EarthCARE (with GK as PI and UF as Co-PI), for the validation of EarthCARE cloud and precipitation products.

RT (3) High-quality solar radiation data

Solar radiation that arrives at the Earth's surface is the key energy input into the climate system. Precise and accurate radiation measurements are therefore of highest importance. For this purpose, the *Austrian Radiation monitoring network* (ARAD) has been established to advance the national climate monitoring and to support satellite retrieval, atmospheric modeling and the development of solar energy techniques. Measurements cover the downward solar and thermal infrared radiation using instruments according to *Baseline Surface Radiation Network* (BSRN) standards. The group runs two of the six ARAD stations (at the University of Graz and at the Kanzelhöhe Observatory), and contributes significantly to this internationally embedded country-wide effort.

RT (4) Historical climate variability

A thorough understanding of natural climate variability is crucial to distinguish anthropogenic climate change. Measurement series are often too short to analyze long-term cycles and changes, and to determine the frequency of extreme events, which have return periods of decades to centuries. In this recent RT, funded by the FWF via the project *Climate History of Central Europe during the Little Ice Age*, we try to obtain a better understanding of natural climate variability by studying historical sources in the pre-instrumental period, and by back-extending time series by previously unprocessed data.

Research Infrastructure

With the high-resolution WegenerNet field facility, comprising about 160 stations in the region around Feldbach in southeastern Austria (1 station per 2 km^2), the University of Graz has a unique climate station measurement network that was founded by GK in 2006. It has recently been further expanded in 2020/21 into the WegenerNet 3D Open-Air Laboratory for Climate Change Research, by adding a weather radar, radiometers, and ground-based GNSS water vapor sensors. This open-air laboratory enables innovative research on weather extremes under climate change and more generally on weather-climate-hydrology-land use changes under climate change. One focus use is, for example, to study small-scale extreme precipitation with previously unattainable accuracy.

The group runs the meteorological station of the University of Graz, which has a long, continuous data series, and was therefore recently awarded by the WMO the prestigious status of a "Centennial Observing Station". A growing database of automated and manual measurements makes the time series increasingly interesting for determine potential offsets in climate data caused by the transition from conventional manual observations to automatic weather stations. The group, represented for this purpose by UF, recently joined the international *Parallel Observations Science Team*.

In close cooperation with the Kanzelhöhe Observatory for Solar and Environmental Research (KSO), which belongs to the University of Graz, an experimental focus has been set on high-precision radiation measurements, and the appropriate measurement infrastructure has been created.

The group works also with data from a large number of satellite missions (RT 1 and RT 2). In the framework of the inter-university *Cooperation Project GEOCLIM Data Infrastructure Austria*, led by GK on behalf of the University of Graz, joint computing and storage capacities for Earth observation and climate research have been and are being established since 2017 in the area of the Earth Observation Data Centre (EODC) and the data services of the Climate Change Centre Austria (CCCA), complemented by high-performance connections to the HPC services of the VSC and ZAMG. These resources are used for IT-intensive analyses and modeling (e.g., of climate, atmosphere, land surface, water balance).

Highlights

In its work in the research theme **RT (1)** the group recently led or co-led ground-braking papers by internationally leading teams in the field of atmospheric climate monitoring, with a focus on temperature trends and global warming, based on radio occultation (RO) and other global observation systems: Steiner et al. (2020) on the consistency of troposphere and stratosphere temperature trends; Von Schuckmann et al. (2020) on the distribution of heat storage from global warming in the Earth climate system; and the proof of the anthropogenic contraction of the stratosphere by Pisoft et al. (2021) are examples of such studies.

Work on the research theme **RT (2)** brought forward, among a series of further topical publications, a recent milestone paper on the WegenerNet data record, achievements, and next steps by Fuchsberger et al. (2020), and a validation of NASA GPM satellite data by Sungmin O et al. (2017).

RT (3): The work by Baumgartner et al. (2018) provided important insight in systematic differences between historic and state-of-the-art measurements of sunshine duration.

RT (4): The temperature record in Graz could recently be extended back to the year 1795, lifting it in the elusive club of continuous time series with a length of more than 220 years. Stangl and Foelsche (2021) found an unexpected high number of historical aurora observations during the "Maunder Minimum" (1645 to 1715) – which is generally regarded as a phase of very low solar activity – and thus responsible for a particularly cold phase during the "Little Ice Age".

The *Atmosphere and Climate Physics Research Group* is not only committed to excellence in research but also in teaching. AS, GK and UF contribute significantly to the success of the *Doctoral Programme Climate Change (DKCC)*. UF recently received the teaching award of the University of Graz („Lehre: Ausgezeichnet!") for the lecture "Introduction to Meteorology and Climate Physics", 2020.

Selected Publications

Baumgartner, … U. Foelsche, and H.E. Rieder (2018) A comparison of long-term parallel measurements of sunshine duration obtained with a Campbell-Stokes sunshine recorder and two automated sunshine sensors, *Theoretical and Applied Climatology*, 133, 263–275, *https://doi.org/10.1007/s00704-017-2159-9*

Fuchsberger, J., G. Kirchengast, and T. Kabas (2021): WegenerNet high-resolution weather and climate data from 2007 to 2020, *Earth Syst. Sci. Data*, 13, 1307–1334. *https://doi.org/10.5194/essd-13-1307-2021*

Pisoft, P., … , U. Foelsche, … et al. (2021), Stratospheric contraction caused by increasing greenhouse gases, *Environ. Res. Lett.*, published online. *https://doi.org/10.1088/1748-9326/abfe2b*

Stangl M. and U. Foelsche (2021) Aurora Observations from the Principality of Transylvania from the 16th to the 18th Century CE, Solar Physics, 296, 78, *https://doi.org/10.1007/s11207-021-01811-7*

Steiner, A.K., F. Ladstädter, … , U. Foelsche, G. Kirchengast, … et al. (2020): Consistency and structural uncertainty of multi-mission GPS radio occultation records, Atmos. Meas. Tech., 13, 2547–2575. https://doi.org/10.5194/amt-13-2547-2020

Sungmin O, U. Foelsche, G. Kirchengast, J. Fuchsberger, J. Tan, and W.A. Petersen (2017) Evaluation of GPM IMERG Early, Late, and Final rainfall estimates with WegenerNet gauge data in southeast Austria, *Hydrol. Earth Syst. Sci.*, 21, 6559-6572. *https://doi.org/10.5194/hess-21-6559-2017*

von Schuckmann, K., … , M. Gorfer, … , G. Kirchengast, … , A.K. Steiner, … et al. (2020): Heat stored in the Earth system: where does the energy go?, *Earth Syst. Sci. Data*, 12, 2013–2041. *https://doi.org/10.5194/essd-12-2013-2020*

Strategic Aims

A very important development in the upcoming 3-year period will be the opening and appointment of a new §98 Professorship on *Climate Physics*, in order to strengthen the Institute of Physics in this field as a key partner in the Field of Excellence *Climate Change Graz*. This new professorship is intended to make optimal use of the available unique research infrastructures summarized above, and to further strengthen the already successful international research cooperation in one or more areas.

A lot of effort has been invested over 2019-2021 into the enhancement of the WegenerNet facilities to their current form as a 3D Open-Air Laboratory for Climate Change Research. The scientific exploitation of this rich dataset in the upcoming 3-year period is hence one of the priority aims that will serve as a core research activity of starting the WegenerNet Open Data and Science Laboratory Region Southeastern Austria as an international research cooperation platform as of 2022.

3.2.3 Didactics

Fachbereich Physikdidaktik & Fachdidaktikzentrum Physik

Science education research is characterised by a broad spectrum of scientific approaches. It deals with teaching and learning processes in the classroom, in the training and further education of teachers, as well as in pre-school and out-of-school learning situations and examines their processes, interrelationships, conditions and results. The aim is to describe what constitutes learning in science in order to improve the quality of teaching and learning processes. The design of research-based teaching-learning arrangements for school settings, teacher education and teacher further education in the paradigm of Design-Based Research (DBR) is one central working field of the Physics Education Research group (PER). DBR is not merely a translation of theory into practice, but a transformation of empirically and theoretically gained knowledge into teaching-learning arrangements which are iteratively tested and refined in order to optimize the performance of the learners and develop domain specific theories about teaching and learning. The outstanding expertise of the PER group in the field of DBR and beyond is internationally renowned. This is reflected in numerous international papers in high quality journals, numerous cooperations with universities and research groups on a national and international level and invitations to prestigious contributions at conferences, in journals and books.

Subject didactic research is conducted empirically using a variety of research methods adapted from the social sciences and psychology. It takes place in close interconnection and productive engagement with teaching practice, as research and development are closely linked. The PER group has substantial expertise in quantitative and qualitative research and vast experience in mixed method scenarios. Science education research is closely linked to subject science, as well as to related disciplines such as educational sciences or psychology. Subject didactic research is therefore per se interdisciplinary or transdisciplinary which is well reflected in the research and cooperation partners of the PER group. Current strands of research are:

Design-Based Research

- Scientific working methods in non-experimental climate physics investigations (upper secondary, teacher education),
- Basic climate change education: teaching/learning scenarios (lower secondary, teacher education, in-service teacher training),
- 3D vision - development of a learning environment for out of school workshops (upper secondary, teacher education, in-service teacher training),
- Graz-Frankfurt optics curriculum: teaching learning environment for optics (lower secondary, teacher education, in-service teacher training),
- EPo-EKo: learning environment for electricity (lower secondary, teacher education, in-service teacher training),
- Promoting diagnostic competence of future physics teachers with focus on students’ conceptions: development of a learning environment (teacher education, in-service teacher training).

Basic Research

- The concept of students’ conceptions and its definition in German speaking physics didactics: Delphi-Study,

- Development of professional competences in physics teacher education,
- Development of concept tests (basic climate change education, simple circuits in electricity).

After its establishment as an individual Fachbereich within the Institute of Physics in 2015, the Physics Education Research group was implemented mid 2017 as a full working group consisting of a principal investigator, a post-doc (100%, fluctuation position, re-staffable), a pre-doc (100%, fluctuation position, re-staffable) and a school-practitioner (50% permanent cooperation position (Dr. Gerhard Rath) till August 2020; in Sept 2020, this position was transformed to a fluctuating 50% lecturer position, re-staffable). The Fachbereich Physikdidaktik has a vast scope of duties in management, teaching, teaching organization (Lehramt Physik, coordination within EVSO (Entwicklungsverbund Süd-Ost i.R. der PädagogInnenbildungNeu)), curriculum work, internal committee work, student counselling and support.

The Covid-19 pandemic is another challenge for the PER group, it causes delays or disables school-related research and development projects, or significantly influences their design and implementation.

The **Fachdidaktikzentrum Physik (FDZ Physik)** is a suborganisation of the Regionales Fachdidaktikzentrum Physik (RFDZ Physik, pdg), a cooperation with the Bildungsdirektion für Steiermark, Pädagogische Hochschule Steiermark and the Katholisch Pädagogische Hochschule Graz. Within the RFDZ cluster, the FDZ Physics is responsible for all administrative and financial issues, for project management and coordination tasks. In addition, it provides the infrastructure for the RFDZ. The FDZ Physics consists of staff from the PER group as well as project staff (MMag. Weiß, MMag. Renner) and cooperating teachers financed by the ministry of Education in course of the IMST Themenprogramm (Mag. Knechtl, Dr. Singer, Mag. Jaritz, Dr. Picher, Mag. Joham). The focus of the FDZ is on school cooperations and continuous professional development (CPD) of science teachers. The transfer of current physics education research results is achieved by in-service trainings, long-term professionalisation programmes, projects with school classes and networking.

Medium-term strategy

In general, the mid-term strategy for the Fachbereich Physikdidaktik is to intensify successful research strands, further deepen and expand cooperation and establish research foci that strategically supplement present research.

This endeavour faces several challenges, especially in the context of third-party funding and human resources: Our present research uncovers several research gaps that may prove very rewarding to pursue in terms of international reputation. However, the current staffing level of the working group is not able to meet the additional amount of research work. On the other hand, the third-party funding situation in the field of subject didactics is not very promising. In addition, the competition for outstanding young researchers in our community makes it also difficult, as there are always attempts to poach researchers who have fluctuation positions.

Assuming a stable staffing situation, most research strands mentioned above will be continued. In addition, focus will be put on four different areas:

- **Digitalisation** in teacher education and physics teaching at secondary level: Learning environments will be developed that support future physics teachers to gain necessary digital competences to be able to transform conventional instruction into meaningful and efficient digital teaching/learning scenarios. Additionally, lesson modules that incorporate digital aspects are developed for school settings, starting with the context of climate change.
- **Inoculation theory as a strategy** to support students in dealing with fake news about science in social media: “Fake news” or misinformation are increasing. Opinion makers on social media tend to guide public discourse on scientific topics more and more, while expert knowledge

falls in the background. A seemingly effective approach to proactively counteract the influence of misinformation is attitudinal inoculation, where learners are provided with the tools / strategies they need to critically evaluate information before encountering (mis)information.

- **Fidelity of implementation & essential features** in educative materials: The development and evaluation of teaching materials and the underlying teaching concepts are a core area of empirical science education research. The question of the fidelity of implementation of such evidence-based teaching materials in the classroom is hardly addressed. A framework model to measure this fidelity of implementation needs to be developed to systematically gain insight into the "black box" of teaching based on teaching materials. Knowing underlying transformation mechanism from the teaching materials and the teaching concept to the enacted teaching behaviour will help to design materials and support systems that help teachers in identifying, accepting and implementing essential and effective features of the teaching materials.

- **Coherence in physics teacher education** with emphasis on mentors and mentoring processes in school practice phases (Pädagogisch Praktische Studien im UF Physik): Practical phases play a central role in the preparation of prospective teachers for their future teaching profession. Results in professionalisation research clearly show that for high-quality teacher education, coherence between school practice and university supervision is an important key element. Currently, there is a lack of knowledge about how teachers act in their role as mentors, which professional facets are supported by mentoring-processes and whether mentors have an appropriate level of professional knowledge to support teacher students in their professionalisation.

Highlights

Since its foundation, the PER group has developed an excellent publication record (publications e.g. in Physical Review Physics Education Research, European Journal of Physics, Physics Education, Journal of Physics, Eurasia Journal of Mathematics, Science and Technology Education, CEPS Journal, …) and increased its international and national visibility. The output of the group is consistently high compared to similar research groups.

In the area of teacher education, a lot of effort (research and development) has been put in the design and evaluation of new and efficient physics didactic courses to provide a physics didactics education on international level. The effort invested in this area is only marginally reflected in typical key figures.

In April 2020, the first dissertation in physics education research was completed. Thomas Schubatzky's dissertation („Das Amalgam Anfangs-Elektrizitätslehreunterricht - Eine multiperspektivische Betrachtung in Deutschland und Österreich") was published by the renowned Logos Verlag in November 2020.

Thomas Schubatzky also succeeded in acquiring third-party funding from the Joachim Herz Stiftung within the framework of the Kolleg Didaktik:digital and he is the first Austrian Fellow in this programme.

After almost three years of post-doc work in the PER group, Ingrid Krumphals was offered the PH1 professorship for Physics Didactics at the University College for Teacher Education Styria.

In the binational project EPo-EKo, in cooperation with the universities of Frankfurt, Darmstadt, Tübingen, Vienna and Dresden, the learning processes of almost 2,000 pupils in the field of electricity were investigated, as were the teaching activities of the corresponding teachers. Ground-breaking findings from this project are being published in renowned journals.

Due to the Covide-19 pandemic, the project has been on hold since spring 2020.

As part of the project on basic climate change education, expert videos have been produced with climate researchers from the Wegener Centre for Climate and Global Change. These videos, together with other research results of the PER group, are part of the currently running exhibition at the Science Centre Welios in Wels (expected 50.000 visitors).

With substantial participation of the PER group, the DINAMA was founded and opened in 2019. It was headed by Claudia Haagen-Schützenhöfer and co-headed in 2021/2022.

The project "IMST Thematic Programme: Competences in Science and Mathematics Education", funded by the Ministry of Education, was extended several times and has raised funds of over 50k plus approx. 0.70 FTE school practitioner for 7 years. The project ends in August 2022 with a successful record of implemented CPD measures and a number of international publications.

In the project "Wissenschaftswerkstatt", a cooperation with the Kaiserschild Stiftung, numerous workshops for Middle School pupils have been developed, implemented and further developed aiming at scientific literacy and interest development of pupils from rural areas and non-academic backgrounds.

The excellent standing of the PER group is underlined by requests to author contributions to renowned university-level textbook series in German-speaking countries (Fachdidaktik Naturwissenschaften, utb; Schülervorstellungen und Physikunterricht. Ein Lehrbuch für Studium, Referendariat und Unterrichtspraxis: Springer; Unterrichtskonzeptionen für den Physikunterricht. Ein Lehrbuch für Studium, Referendariat und Unterrichtspraxis: Springer Spektrum) and to author international high-level anthologies (International Handbook on Physics Education Research – currently in progress).

Claudia Haagen-Schützenhöfer was awarded the Josef Krainer Gedenkpreis for her habilitation.

Claudia Haagen-Schützenhöfer is permanent co-editor of Plus Lucis, the only Austrian physics and chemistry didactics journal. Plus Lucis contributes to bridging the theory/research – practice gap.

The University of Graz is represented in the ministerial expert group for the new lower secondary school curriculum by Claudia Haagen-Schützenhöfer. As well as in the ministerial expert committee for physics school-textbooks.

3.2.4 Theoretical Particle Physics

Status

The overall structure of theoretical particle physics is defined by its doctoral academy, in which the permanent staff as well as temporary junior research groups participate. It is a follow-up structure to the FWF funded graduate school. As a common structure it is build on the common core competence, which makes this unit unique, the intertwined use of first-principle, genuinely non-perturbative approaches to quantum field theories. It is a declared aim to maintain this unique characteristic, and at the same time cover a wide range of applications. This allows to cover in both undergraduate and PhD level education the full breadth of modern fundamental physics. This common structure was recently excellently reviewed, and its continuation recommended by an international review board.

This current status is the consequence of a strategic development over the last eight years. In this time the relatively focused application area of strong interactions physics has been consecutively expanded, both due to hiring decisions as well as by applied and funded projects, and by unlocking new fields by the members. By this, the current breadth covers applications of particle physics methods in solid state physics, strong interactions, high-energy physics, astroparticle physics to quantum gravity. This is documented by both publications as well as funded projects. In the end, all of these diverse seeming topics are tied to a methodological core, which connects everyone within the unit, giving a common structure.

This allowed to branch out substantially in the last few years to establish new research networks within Austria. Most prominent examples among them are the joint research group on strongly-interacting dark matter with the ÖAW institute HEPHY in Vienna, active participation in various COST networks on particle physics, common proposals for SFBs with essentially all theoretical and experimental groups in Austria, and editorship for the theory section of the Austrian input to the European Strategy on Particle Physics. This development for a stronger cooperation as a particle physics network Austria is also documented by a common yearly retreat, which includes strategic planing sessions, as well a jointly organized conferences, like the ALPS series or the bids for the Higgs conference 2022 and for the Flavour Physics and CP Violation conference 2023 in Vienna.

These national activities are sided with international ones, ranging from individual cooperations, joint conference, and conference series, organization, joint structured research programs and application for them, up to managing positions in international COST networks.

Highlights

A few recent highlights from this research group are:

- The newly-established group of Prof. Sexty showed how to generalize improved gauge and fermionic actions to the Complex Langevin framework. With this, it was possible to extend the investigations of the QCD phase diagram, up to unprecedented densities, finding its equation of state up to about a quark-chemical potential four times as high as the temperature. At lower ratios, where other methods could still yield reliable results, agreement was demonstrated. This gave a first-principle calculation of the densest fermion system found in nature. The developed techniques are, in principle, also applicable to other dense fermion systems. This is shown in illustration 1.
  Phys. Rev. D100 (2019), 074503

- The group of Prof. Alkofer has, in order to understand the quarks' masses and mixing patterns, explored the simplest possible parameterisation of new physics that results in an ultraviolet complete gauge-quark sector of the Standard Model. This ansatz gives rise to an intricate web of Renormalization Group fixed points, and it provides predictive power with respect to the flavour structure and mixing patterns, which we investigate to demonstrate that some of the free parameters of the Standard Model could be determined by the Renormalization Group flow
  Annals of Physics 421 (2020) 168282.

- The junior research group of Dr. Sanchis-Alepuz calculated, and for higher-lying states predicted, the glueball spectrum using a parameter-free fully self-contained truncation of functional equations in Yang-Mills theory. The results are in good agreement with corresponding ones from lattice QCD, where available. This first-principle computation of gauge-invariant states marks a major breakthrough in functional approaches to QCD.
  Eur. Phys. J C 80 (2020) 1077.

- A new hidden symmetry, which is a symmetry of the color charge of quantum chromodynamics, was discovered in the group of Prof. Glozman. In collaboration with Japanese Lattice QCD this symmetry was observed in QCD correlation functions at temperatures that are relevant to experimental studies of hot QCD matter at BNL and CERN. This implies that the hot QCD matter at temperatures below 500 MeV is not a quark gluon plasma, but rather a matter where the degrees of freedom are chirally symmetric quarks connected by the electric string. A consequence is shown in illustration 2.
  Phys. Rev. D 100 (2019) 014502 and Phys. Lett. B 802 (2020) 135245.

- In a collaboration between theoreticians, phenomenologists, and experimentalists from Vienna and Graz, the group of Prof. Maas discussed the possibility of having a larger Higgs contribution in the proton than usually assumed, and how it could be accessed in experiments like the CMS at CERN. it was shown that this is compatible with existing data, and should be likely accessible within the next ten years of LHC run-time at CERN. This result also was taken up by a variety of national media, e.g. the ORF. An example is shown in illustration 3.
  Phys. Rev. D101 (2020), 114018.

Future

Theoretical particle physics is one of the eight core areas of the future GCP, and in addition contributes to the core area of computational physics. The strategic aim is to maintain as the common characteristic the usage of genuine non-perturbative first-principle methods in particle physics, both analytically and computationally. This will carry over the characteristic of the research unit to the GCP, and will maintain the national and international unique orientation. As recommended, the continuation of the doctoral academy as the common frame is a declared goal.

At the moment, the strategic development is at a crucial point, with about half of the core research area retiring in a period of less than five years, with one professorship not to be refilled. While this substantially slows down existing activities, this is a boon in the continuation of the strategic reorientation of this core research area to cover the most relevant research areas in fundamental physics in the future.

In this context, a strengthening of contacts to the particle physics experiments in Austria will be a decisive element. This will be especially emphasized in the follow-up to Prof. Schweiger, which will be opened in 2021. The aim is to fill the position with someone establishing explicit cooperation with experiments in hadron physics and flavor physics in which Austria participates, i.e. Belle II, CMS, ALICE, or the low-energy hadron program of the SMI. In particular before the backdrop of recent discoveries, e.g. about 60 new hadrons at CERN alone as well as tantalizing hints for universality violations for flavor physics mounting since a decade, a strengthening of this field in Graz promises a substantial impact.

This complements our continuing activities on strong interaction physics, which focus besides hadron physics on the phase diagram of the early universe and dense stellar objects, as well as their recreation in heavy-ion experiments. These questions are continuously and vigorously pursued into the future by Profs. Gattringer, Glozmann, and Sexty. Especially with the experimental exploration of new states of matter in context with the ALICE experiments, as well as other facilities like BNL, and with gravitational wave astronomy, this field has a bright future. Moreover, many of the algorithmic developments are highly relevant in interdisciplinary research with solid state physics or quantum chemistry. It will therefore continue to be an important aspect of research.

On longer time scales the successor to Prof. Alkofer in 2023-2025 is aimed to extend the new field of applying the core methods to astrophysical applications, e.g. in terms of compact stellar objects, in accordance with the research of Profs. Gattringer and Sexty, or astroparticle physics of the FWF-funded research group, or quantum gravity as pursued by Prof. Maas. This will cover one of the most active areas of contemporary particle physics. Especially astroparticle physics would provide further opportunities to link to experimental groups in Austria.

Finally, great effort will be invested to create and participate in a national research network on particle physics, e. g. as a cluster of excellence, as a platform to have substantial weight in this very international research area. This will especially apply to strengthen ties to experimental research in particle physics, also in line with the Austrian Ministry of Science’ FIT strategy, as well as the digital initiative at the University of Graz. This will also strengthen the computational physics core area of the future GCP aside from the already existing integral part in simulations methods. A primary path will be by continued common applications to structured research programs. E.g. at the time of writing with a proposal for an SFB on top and Higgs physics at LHC/CERN jointly with experimental and theoretical groups in Vienna.

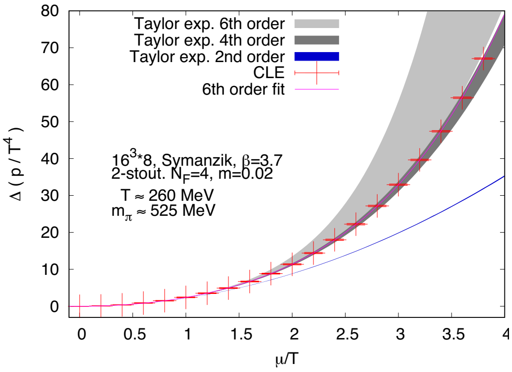


Illustration 1: Results on the QCD pressure as a function of ratio of chemical potential to density from a novel approach to dense fermion system.

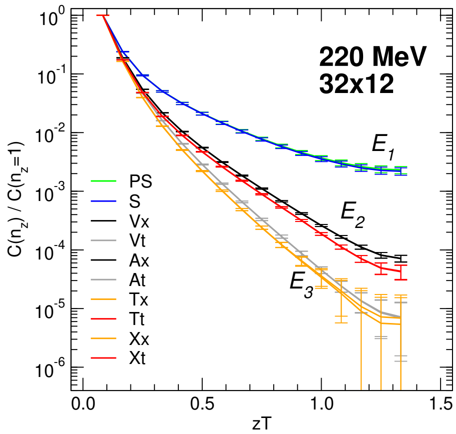


Illustration 2: The discovered unexpected degeneracy patterns in the hadron spectrum above the phase transition, which indidcate teh existence of new, qualitative features of matter in this temperature region.

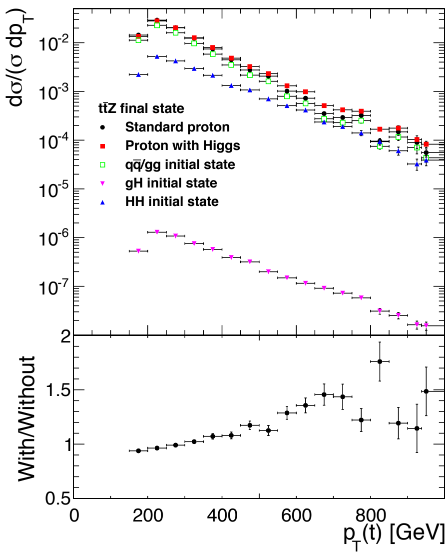


Illustration 3: Prediction for the consequences of the Higgs content of the proton for the CMS experiment at CERN

Ultimately, this strategy continues the pathway started about 8 years ago, to diversify the applications of a common framework, and integrate particle physics in Graz into a strategically developed particle physics community in Austria.

The GCP and the Universities in Graz will profit from this especially in terms of computational physics and an exchange of methods on aspects like dense fermion systems, non-equilibrium physics, large-scale high-performance computing and simulation techniques, big data analysis and eventually applications like machine learning.

3.3 Computational Physics

Computational physics activities are pursued in the research groups "Astro- and solar physics", "Physics of atmosphere and climate", "Theoretical particle physics", and "Theoretical solid state physics". The primary tool are the local HPC clusters, as well as the VSC, and thus members of this groups are also part of the HPC user group. In this form, they contribute to the development of the HPC resources at the University in Graz, as well by adding resources depending on funding. As this is the major infrastructure for theoretical research, these activities are supported by the institute using infrastructure resources.

Particular highlights can be found in the corresponding research group entries. It should only be added that also the development of numerical algorithms is part of the corresponding research activities. This is documented by publications in pure computational science journals. Thus method development and application move coherently.

Most of the development in this area is with respect to simulations algorithms, ranging from conventional numerical linear algebra up to machine learning applications. In the past, this was mainly done on standard CPU systems, but a strategic investment into a GPU cluster has been decided upon and will be implemented in 2021. In addition, several of the professorships to be refilled within the next few years, most notably those in "Astro- and solar physics" and "Theoretical particle physics", are expected to be more computing intensive than previously. This is a natural development based on computational physics becoming more and more relevant in research. This is implementing also the digitalization initiative of the University of Graz. In this context, long-term strategies for code development and maintenance for the purpose of reproducibility will be a major goal. This will be partly implemented by the use of permanent senior scientist positions, who guarantee a sufficiently long-term perspective. In addition, suitable infrastructure, like versioning systems and public interfaces for open data, are important development goals. The aim is to make simulations, and simulation results, openly accessible and document. This is especially important to meet the demands of funding agencies in this respect.

General Services

4. General Services

Administration

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