

Integrative Research Institute for the Sciences Biennial Report 2019/2020

ADLERSHOF

PREFACE

IRIS Adlershof has significantly strengthened and expanded its position as an internationally recognized and highly visible player in the fields of hybrid inorganic and organic systems for optics and electronics, as well as for the physics of space, time and matter.

In particular, large collaborative projects such as the Collaborative Research Center 951 as well as BMBF and EU projects have been pursued, ERC-projects have been awarded and major meetings and conferences have been hosted. Internationally, in addition to its long-term strategic partners in the US and Asia, Princeton University and the National University of Singapore, IRIS Adlershof established a formal cooperation with the Institute of Physics of the Chinese Academy of Sciences.

These successes were enabled through the major improvement of the spatial and technical infrastructure that went hand in hand with the successful completion and the gradual commissioning of the IRIS research building towards the end of 2020. About 2,500 m2 of state-of-the-art laboratory space



and 2,200 m2 of office and common rooms are now additionally available for the research at IRIS Adlershof and for collaborations with our national and international scientific partners. The federal government, the state of Berlin, and Humboldt-Universität zu Berlin provided a total of 53 million ϵ for this purpose.

Moreover, IRIS Adlershof has also expanded its research areas into new directions, including Big Data, Quantum Technology and Catalysis. Here, IRIS members are actively involved into the establishment of new large collaborative projects.

Altogether, IRIS Adlershof looks gladly back on its successes during the reporting period, which also includes growing recognition in the international community, reflected in increasing numbers of invited lecturers at internationally significant conferences as well as highly recognized publications.

All of the above has only been possible through the collaboration of all of the IRIS-members together the early-career researchers at IRIS Adlershof. The promotion of the latter has been a strong focus from the very beginning, strengthened recently by the introduction of a new doctoral program in each IRIS research area - the Advanced Materials graduate school in the research area Hybrid Systems for Optics and Electronics and the RTG 2575 in the research area mathematics - physics of space-time matter.

It is my pleasure to thank all members, their associates, as well as the staff of IRIS Adlershof for their dedicated work, and we are all very grateful for the support that we have received from the administrative departments and the President's office of Humboldt-Universität zu Berlin. Certainly, we are very much looking forward to further fruitful collaborations.

Sincerely,

Prof. Jürgen P. Rabe

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1. EXECUTIVE SUMMARY

The Integrative Research Institute for the Sciences, IRIS Adlershof, drives innovation through interdisciplinary cuttingedge research, with a strong focus in the physical sciences, and with potentially high impact on technology and society at large. It aims at a successful competition within the next round of the Excellence Strategy. IRIS Adlershof will therefore strengthen its interdisciplinary research in its core research areas, and develop and exploit the potential provided by its new IRIS Research Building. Moreover, cooperations will be developed further: Particularly within the Berlin University Alliance (BUA), with its partners of the Helmholtz Association, the Max Planck Society, and the Leibniz Association, as well as with its international partners.

At IRIS Adlershof, outstanding scientists, primarily associated with disciplinary institutes, are provided with pertinent excellent scientific infrastructure, including state-of-the-art equipment, and a dedicated service-oriented IRIS office. Particular emphasis is put on the support of junior research group leaders and early-career researchers: High potentials for science and innovation obtain excellent education and room for development. The research program is based on two main research areas: Hybrid Systems for Optics and Electronics and Mathematical Physics of Space-Time-Matter. Their development, as well as the recently introduced three further research areas, Big Data, Quantum Technology, and Catalysis, determined the work of IRIS Adlershof in the reporting period. Together with cultural science, the epistemology of experimental systems is addressed across the research areas.

Evidence for the successful work in the reporting period includes the about 50 third-party funded projects acquired by IRIS Adlershof's scientific members and associated junior research group leaders, leveling about 24 million Euros. The annual number of scientific publications has grown to more than 180 in 2020, to a significant part in high-impact journals including Science, Nature, Nature-Family, Phys. Rev. Lett., Phys. Rev.-Family, J. Am. Chem. Soc., Angew. Chem., Chem. Soc. Rev., Adv. Mater., Adv. Mater.-Family, JHEP, and Phys. Lett B. Correspondingly, the citation rate has increased to over 9.000 in 2020. The IRIS Research Building, dedicated to the research area *Hybrid Systems for Optics and Electronics*, was completed in the current reporting period and is currently commencing operation. Its funding, provided jointly by the federal and state governments as well as HU, was acquired by IRIS

Adlershof. It totals about 53 million Euros for about 4.700 m² dedicated lab-, office-, and meeting space, including about 10 million Euros for large-scale scientific instruments and equipment.

The cooperation within HU, as well as with the other universities in the Berlin/Brandenburg region, takes place mainly within the framework of large collaborative, third-party funded projects. Funding for the core project of the research area *Hybrid Systems for Optics and Electronics*, the Collaborative Research Center (CRC) 951 *HIOS* (spokesperson N. Koch, IRIS Adlershof), was secured for another four years during the current IRIS reporting period. In addition, IRIS Adlershof plays a leading role in the European Cluster of Excellence *NOMAD* as well as in several other EU-funded projects (*HI-ACCURACY*, *UHMob*, *SAGEX*). The engagement in the *Innovation Network for Advanced Materials* (*INAM*) in Berlin aims at the development and the implementation of innovative concepts for the application of novel materials and technologies in electronics, optics, and photonics. Moreover, two new *Joint Labs* were set up and are operated jointly with non-university research institutions. IRIS Adlershof is also involved in the Excellence Strategy of the federal and state governments as an integral part of the BUA. This includes the collaboration of IRIS Adlershof with the Clusters of Excellence *Matters of Activity*. *Image – Space – Material*, *UniSysCat*, and *MATH+*.

The promotion of early-career researchers is enhanced through institutional and third-party funded actions. Particularly noteworthy are the *Graduate School Advanced Materials* of HU (spokesperson N. Koch, IRIS Adlershof) and the recently established DFG-funded Research Training Group 2575 *Rethinking Quantum Field Theory* (spokesperson J. Plefka, IRIS Adlershof), which are in the core of the IRIS research areas *Hybrid Systems for Optics and Electronics* and *Mathematical Physics of Space–Time–Matter*, respectively. Further research and training actions for early-career researchers include Max Planck Research Schools and EU-funded Innovative Training Networks.

IRIS Adlershof is a place of diversity, plurality of opinion, equal opportunity, mutual appreciation, and respect. As one example, the underrepresentation of female scientists, which is still widespread especially in mathematics and physics, was counteracted by targeted support for young female scientists.

The international visibility of IRIS Adlershof and the radiance of HU's Campus Adlershof have increased significantly during the reporting period. IRIS Adlershof's members gave a large number of invited lectures at international scientific events, enjoyed research stays abroad, hosted visiting researchers, and organized several scientific workshops and conferences. Particularly vivid was the exchange with Humboldt-Universität's strategic partners Princeton University and the National University of Singapore. The already existing collaboration with the renowned Institute of Physics of the Chinese Academy of Sciences IOP/CAS was very recently raised to a new level by signing a *Memorandum of Understanding* and starting a joint PostDoc program.

2. STRUCTURE AND INSTITUTIONAL FUNDING

2.1. IRIS Adlershof within the University Structure

HU, according to its constitution, consists of faculties and departments, other scientific institutions, central service institutions, and central management and administration. The Charité - Universitätsmedizin Berlin is operated as a joint faculty of both, Humboldt-Universität zu Berlin and Freie Universität Berlin. Five of HU's faculties consist of different scientific departments, the remaining three are mono faculties. The Faculty of Mathematics and Natural Sciences consists of the Departments of Chemistry, Computer Science, Mathematics, and Physics.

Integrative Research Institutes – An Innovative Research Format at HU

The development of the format of an Integrative Research Institute (IRI) was one of the priorities of HU's Institutional Strategy *Educating Enquiring Minds. Individuality – Openness* – *Guidance* that was funded through the Excellence Initiative from November 2012 to October 2019. IRIs are interdisciplinary institutes, promoting collaborations with a strong research focus and thus play a decisive role in developing HU's profile. At the same time, by encouraging close collaborations also with external research partners, IRIs are means to exploit potential at the interface between HU and non-university research, and also of developing collaborative research at HU over the long term.

IRIS Adlershof as a Builder of Bridges

The prototype of this new research format, IRIS Adlershof, was established through nine professors in 2009. Its main goal is to provide its scientists with an excellent infra-structure for joint research in natural sciences. This is by providing a high-quality research infrastructure including state-of-the-art equipment, as well as through financial or administrative resources provided by a service-oriented IRIS office. IRIS Adlershof is a kind of *bridge builder*, pursuing an

interdisciplinary approach to develop new scientific directions and new methods of interdisciplinary cooperations. At the university level, IRIS Adlershof, therefore, brings together scientists from the HU's Departments of Chemistry, Computer Science, Mathematics, and Physics. IRIS Adlershof also promotes the connection between HU's natural and cultural sciences, and between theory and experiment, by close research collaborations with colleagues from other institutes, particularly within the Cluster of Excellence Matters of Activity. Image - Space - Material. Regarding HU's infrastructure. IRIS Adlershof thus also functions as a link between the university campuses Adlershof and Mitte. The new IRIS Research Building (see Chapter 3.3.1) also reinforces the idea of IRIS Adlershof as a bridge builder, since it provides the infrastructural basis for approaching scientific problems from different perspectives, from physics and chemistry, from mathematics and physics, as well as from theoretical and experimental perspectives.

Located in Germany's leading science and technology park, IRIS Adlershof builds bridges not only within HU but it also acts as a link to non-university research institutions with a strong focus on application, as well as to commercial enterprises to promote the transfer of knowledge between research and practice. *E.g.*, innovative high-tech enterprises and research institutions are invited to send their personnel to work on specific projects in jointly operated laboratories. With this concept, the collaboration between IRIS Adlershof and pertinent scientific and industrial partners is to be promoted in the long term. For more details, see Chapter 4.

2.2. INNER STRUCTURE OF IRIS ADLERSHOF

2.2.1. GOVERNING BODIES

IRIS Adlershof is an institute according to §25 of HU's constitution. Its main governing bodies are the General Assembly, the Council, and the Director, which are all supported by the IRIS office.

The **General Assembly** is the highest body of IRIS Adlershof. It elects the Director and the other members of the Council, and advises on the thematic, conceptual, and infrastructural development.

The **Council** decides on all important matters of IRIS Adlershof that do not fall within the remit of other authorities of the HU, including the appointment of new IRIS Adlershof members.

The **Director** leads the current business, represents IRIS Adlershof internally and externally, leads the meetings of the General Assembly and the Council, and is bound by their decisions within the scope of their respective competences. The Director must be a university professor at HU.

The **IRIS Office** is responsible for all administrative matters of IRIS Adlershof. It is not only the interface to the local and



central administrative bodies of the university, but as a central service-oriented institution it supports all bodies of IRIS Adlershof, particularly the members. This is important since the members originate from different institutes and institutions. The IRIS office manages the resources of IRIS Adlershof and provides administrative support, *e.g.*, for applications for third-party funding, in organizing and realizing

CURRENT ELECTED MEMBERS OF THE IRIS COUNCIL



Jürgen P. Rabe (Director)

Humboldt-Universität zu Berlin, Department of Physics & Max Planck Institute of Colloids and Interfaces scientific events such as the international conference F π 14, and in managing the promotion of early-career researchers. In this way, the researchers at IRIS Adlershof are relieved of administrative requirements to a certain extent and can therefore concentrate better on their central tasks: scientific research and teaching.



Norbert Koch (Deputy Director)

Humboldt-Universität zu Berlin, Department of Physics & Helmholtz-Zentrum Berlin für Materialien und Energie GmbH



EMIL LIST-KRATOCHVIL

(DEPUTY DIRECTOR AND HEAD OF COMMISSION RESEARCH BUILDING)

Bridging Professorship Physics/Chemistry

HU Berlin, Departments of Physics and Chemistry & Helmholtz-Zentrum Berlin für Materialien und Energie GmbH



MATTHIAS STAUDACHER

Bridging Professorship Physics/ Mathematics

HU Berlin, Departments of Physics and Mathematics



Julian Miczajka, M. Sc.

(Early-Career Researchers Representative)

HU Berlin, Department of Physics & Max-Planck-Institut für Gravitationsphysik (Albert-Einstein-Institut)

2.2.2. **Members**

IRIS Adlershof consists currently of 24 regular members. In addition, three junior research group leaders and about 140 early-career researchers (graduate students, postdocs) are associated with IRIS Adlershof.

The members of IRIS Adlershof are university professors or postdoctoral associates with outstanding achievements in the IRIS research areas and/or competence fields. Due to IRIS Adlershof's interdisciplinary and integrative concept, they belong to different scientific departments of HU or other universities, namely the Departments of Chemistry, Computer Science, Mathematics, and Physics.

LINK TO NON-UNIVERSITY PARTNERS

IRIS Adlershof is also closely linked to non-university research institutes through its members. This includes institutes of the Max Planck Society (Max Planck Institute of Colloids and Interfaces (MPI-KG), and the Fritz Haber Institute of the Max Planck Society (FHI), the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), and several institutes of the Leibniz Association (Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI), the Zuse Institute Berlin (ZIB), and the Weierstrass Institute for Applied Analysis and Stochastic (WIAS). An overview of all partner institutions can be found in chapter 4.

New Members Appointed During the Reporting Period

During the reporting period, IRIS Adlershof has appointed two new regular members (see below), who will strengthen IRIS by contributing to its further expansion and also interlinking the research areas of IRIS Adlershof:

The appointment of Olaf Hohm in 2019 has been an important addition to theresearch area *Mathematical Physics* of *Space-Time-Matter*. Hohm leads the ERC Consolidator Group *Symmetries and Cosmology*. He is developing a computa-



Olaf Hohm



Tim Schröder

tional approach based on string thearguably the ory. most promising candidate for a complete theory of quantum gravity. This approach might answer questions relating to the very early history of the universe, and even test string theory on measurements of background radiation.

In 2019, Tim Schröder was appointed a new member of IRIS Adlershof to strengthen the field of competence *Modem Optics*. He is researching quantum amplifiers with the ERC project *QUERP - Quantum Repeater Architectures Based on Quantum Memories and Photonic Encoding* and is also trying to combine complementary technologies from quantum communication.

EXTERNAL CALLS AND OFFERS

During the reporting period, four members of IRIS Adlershof received and accepted external calls for permanent academic positions (see table below). However, all of them are still linked at HU for at least 20% of their working hours and decided to continue their engagement as a member of IRIS Adlershof.

Offered to	Offering Institution	Offer	Year
Setfan Hecht	RWTH Aachen & Leib- niz Institute for Interactive Materials (DWI)	W3-Profes- sorship & Scientific Di- rector	2019
Matthias Ballauff	Freie Universität Berlin	Guest Pro- fessorship	2019
Catherina Cocchi	Carl von Ossietzky Universität Oldenburg	W3-Profes- sorship	2020
Michael J. Bojdys	Kings College London	Reader in Chemistry	2020

2.3. INFRASTRUCTURE OF IRIS ADLERSHOF

2.3.1. IRIS RESEARCH BUILDING

The successful completion and the gradual commissioning of the new IRIS Research Building in late 2020 have been a highlight. The Research Building is dedicated to the research area Hybrid Systems for Optics and Electronics and it improves significantly IRIS Adlershof's lab facilities and scientific infrastructure. Previously, the infrastructure did not allow for highly specialized laboratories to be set up in the existing IRIS Adlershof building at Zum Großen Windkanal. Instead, the experimental groups had to use remote laboratories in their respective departmental institutes. The completion of the Research Building is therefore a major improvement for IRIS Adlershof. With the Research Building, IRIS Adlershof offers its members excellent working conditions through its new laboratories and the provision of high-end, state-of-theart equipment. By providing joint labs, IRIS Adlershof enables research, which could not be performed in the disciplinary departments of physics and chemistry.

IRIS RESEARCH BUILDING FOSTERS IRIS' INTEGRATIVE CONCEPT

The IRIS Research Building comprises 2,500 m² of laboratory space and 2,200 m² of office space and common rooms. In its center, the building provides laboratories of different sizes and specializations, ranging from standard physics laboratories with common media supply and wet laboratories with two or more hoods, to clean rooms and high-quality optical laboratories with controlled and stable climatic conditions to magnetically shielded and vibration-decoupled. The basement provides laboratories with high-end vibration isolation and magnetic shielding for state-of-the-art transmission electron microscopy (TEM). The offices are located in the immediate vicinity of the laboratories, offering space for more than 160 desks.

2.3. Infrastructure of IRIS Adlershof



To provide opportunities for fruitful informal discussion and exchange, the laboratories and offices are located close to each other, but at the same time are separated by membrane-like common areas. Researchers from different fields, such as physicists and chemists, or theoreticians and experimentalists can thus interact more closely with each other. Several seminar rooms are available for discussion, presentation, and lectures. The entrance area itself is designed to provide space for poster presentations, which makes this building very suitable for conferences. The interdisciplinary approach of IRIS Adlershof is therefore not only reflected in the structure of the new Research Building, but interdisciplinary cooperation and communication are also being fostered.

LABORATORIES AND INSTRUMENTATION

The new laboratories provide access to state-of-the-art scientific instrumentation, which enable a broad range of fabrication and characterization methods, including wet and vacuum methods, printing, as well as a broad range of spectroscopies and microscopies, both in- and ex-situ. An outstanding device is the NION high-resolution TEM with an ultrahigh resolution energy filter, which is a very powerful tool for the investigation of organic and inorganic structures down to the atomic scale, allowing also for vibrational spectroscopy of molecules. It is supplemented by other TEMs, including a cryo-TEM and scanning electron microscopy. Moreover, the IRIS Research Building offers devices for photo- and electron-beam-lithography within the cleanroom, a 19 m long glovebox cluster, an ultra-high vacuum (UHV)cluster, and scanning probe devices, such as atomic force microscopes and force robots, in close proximity. Numerous wet labs offer plenty of workspace in BIO-S1 and BIO-S2 certified settings, and measuring rooms of different sizes and qualities provide space for short-, mid-, and long-term research in single usage- or coop-space.

Results

The successful commissioning of the Research Building was a central milestone for IRIS Adlershof. The building will promote the implementation of many of the institute's goals. On the one hand, the infrastructural basis for the research of IRIS Adlershof will be strengthened. On the other hand, the conditions for new cooperations with national and international partners from science and industry at the Adlershof site will be significantly improved. For example, an innovative research laboratory devoted to research on Thin Films as Catalysts and operated jointly, together with the HelmholtzZentrum Berlin für Materialien und Energie (HZB) and the Fritz Haber Institute of the Max Planck Society (FHI), will be based in the new IRIS Research Building. At the end of the

2.3.2. JOINT LAB FOR STRUCTURAL RESEARCH

IRIS Adlershof runs a core facility, which is available not only to its members but also to its cooperation partners: The *Joint Laboratory for Structural Research (JLSR)* provides and develops infrastructure and equipment for structural research on organic, inorganic, and corresponding hybrid materials and systems. It focuses on microscopy, scattering, and lithography using electrons, X-rays, and scanning probes. The JLSR was established as a joint institution of the HU, the HZB,

2.4. INSTITUTIONAL FUNDING

IRIS Adlershof receives 200.000 Euros p.a. basic funding from central HU resources, to cover its personnel costs for the IRIS office. Within a 91B-GG-procedure, IRIS Adlershof raised national and state funds required for the construction of the Research Building amounting to approx. 53 million Euros. For instrumentation, further funding was allocated by reporting period the colleagues have been moving in and assembling the laboratory equipment required to carry out the project The experiments will begin within 2021.

and the TU Berlin under the roof of IRIS Adlershof. The commissioning of the IRIS Research Building significantly expands the infrastructure available for the *JLSR*, namely through the additional high-end transmission electron microscopes available there. In this way, the JLSR shall be developed to a Berlin-wide *Joint Lab for Microscopy* together with HZB and with the FHI as a new partner.

HU's institutional strategy that has been funded through the Excellence Initiative until October 2019.

The research is largely financed through third-party funding, including DFG, EU, BMBF, AvH, Volkswagen Foundation, and within the framework of institutional collaborations.

3. RESEARCH

IRIS Adlershof builds on the particular competences of HU in the fields of *Modern Optics*, *Molecular Systems*, *Mathematical Physics*, and *Computation in the Sciences*. Each of these

3.1. MAIN RESEARCH AREAS

IRIS Adlershof has focused from its beginning on two main areas of research: *Hybrid Systems for Optics and Electronics* and *Mathematical Physics of Space–Time–Matter*.

HYBRID SYSTEMS FOR OPTICS AND ELECTRONICS

Hybrid inorganic/organic systems structured on atomic, molecular, and mesoscopic length scales provide completely new opportunities for the implementation of optical and electronic properties and functions, approaching fundamental limits. Based on physico-chemical concepts and inspired by the extraordinary efficient way functions are implemented in natural systems, the structure-property relationships of these novel hybrid materials are investigated and explored for their application potential. competence fields encourages close cooperation across the interdisciplinary boundaries of physics, chemistry, mathematics, and computer sciences.



Organic molecules on a semiconductor – animation from "HIOS – The Movie"

MATHEMATICAL PHYSICS OF SPACE-TIME-MATTER

Modern physics strives to understand from first principles the structure of space, time, and matter on very large and very small scales, as well as in complex systems. An important and challenging objective is to analyze the role of basic symmetries as well as the way they are broken. The ultimate goal is to find the Weltformel, to describe the fundamental forces and their interactions by a sincoherent theory. gle Hopefully, it will become clear along the way how the smooth world that we expe-



rience emerges from the *chaotic* principles of quantum physics. Mathematicians and theoretical physicists are coop-

erating to address specific questions of mathematical physics in the described framework.

3.2. Key Developments in Research

IRIS Adlershof's goals in the reporting period were to expand interdisciplinary research in its two research areas and to identify the potential for new research fields. Consequently, IRIS Adlershof also focused on expanding existing and establishing new research collaborations with national and international partners, both within and outside the university.

3.2.1. IRIS Adlershof in the Excellence Strategy

IRIS Adlershof participateds intensely in Clusters of Excellence and Graduate Schools in the Excellence Strategy by the federal and state governments.

EXC 2008: Unifying Systems in Catalysis – UniSysCat



IRIS Adlershof is involved in UniSysCat (spokesperson A. Thomas, TU Berlin) through its members

S. Hecht and C. Limberg. *UniSysCat* works in five interdisciplinary research areas on the elucidation and evolution of catalyst networks. The central scientific objective is to master the next stage of future challenges in catalysis: how to elucidate, create, and control reaction networks in chemical and

biological catalysis at different levels of complexity in space and time. *UniSysCat* is involved in a variety of national and international collaborations. The core group of *UniSysCat* with four universities in Berlin and Potsdam, FHI, and the MPI-KG has collaborated for more than ten years in *UniCat* and a number of CRCs. New partners of the consortium are the Charité – Universitätsmedizin Berlin with its expertise in structural biology, the Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), contributing its NMR facilities and expertise, and the HZB, including its synchrotron source BESSY II, a particularly important infrastructure for developing new approaches in protein spectroscopy and the *in situ* analysis of catalytic processes.

EXC 2025: MATTERS OF ACTIVITY. Image – Space – Material

Through its members J. P. Rabe (also as a board member of Matters of Activity) and M. Staudacher, IRIS Adlershof is involved in the cluster Matters of Activity (spokesperson W. Schäffner, HU). The cluster aims at a basis for a new culture of materials. The central vision of the cluster is to rediscover the analog in the activity of images, spaces, and materials - and in the age of the digital. Biology and technology, mind and material, nature and culture intertwine in a new way. In this context, the interdisciplinary research and development of sustainable practices and structures is a central concern in areas such as architecture and soft robotics. textiles, both materials and digital filters, and surgical cutting techniques. In six projects, more than 40 disciplines systematically investigate design strategies for active materials and structures that adapt to specific requirements and environments. The cluster focuses on a new role of design, which is emerging in the context of growing diversity and the continuous development of materials and visualization forms in all disciplines. Among the cooperation partners are the Charité - Universitätsmedizin Berlin, FU Berlin, HTW University of Applied Sciences Berlin, MPI-KG Potsdam, the Museum of Decorative Arts, State Museums of Berlin, Prussian Cultural Heritage Foundation, TU Berlin, and weißensee school of art berlin.

EXC 2046: MATH+: Berlin Mathematics Research Center

Berlin Mathematics Research Center

MATH+ is jointly led by IRIS Adlershof member M. Hintermüller, C. Schütte (FU

Berlin), and M. Skutella (TU Berlin). J. Kramer from IRIS Adlershof is also involved as a board member. *MATH+* is a cross-institutional and transdisciplinary Cluster of Excellence. It sets out to explore and further develop new approaches in application-oriented mathematics. Emphasis is placed on mathematical principles for using ever-larger amounts of data in life and material sciences, in energy and network research, and in the humanities and social sciences. *MATH+* is funded by the DFG for a first period of seven years since January 2019. It is a joint project of the three major universities in Berlin (HU, FU, TU) as well as the WIAS and the ZIB. *MATH+* continues the success stories of the renowned Research Center *MATHEON* and the Excellence Graduate School *Berlin Mathematical School* (BMS). HIOS

3.2.2. RESEARCH AREA HYBRID SYSTEMS FOR OPTICS AND ELECTRONICS

CRC 951: Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS)

The involvement of IRIS Adlershof in the CRC is very high: *HIOS* is headed by the two IRIS members N. Koch (spokesperson) and O. Benson (deputy spokesperson), and a total of nine IRIS members participate as PIs. *HIOS* is the lighthouse project of the

IRIS Adlershof research area *Hybrid Systems for Optics and Electronics*. The CRC has a strong scientific impact on hybrid systems that unite inorganic semiconductors, conjugated organic materials, and metal nanostructures. The CRC's goal is to realize substantially improved and potentially novel optoelectronic functionalities that are not achievable with any of the individual material classes alone. During the years under review, IRIS Adlershof focused on the preparation of its third funding period, which was approved in May 2019 by the DFG. Important cooperation partners are the TU Berlin, the University of Potsdam, HZB, and the FHI.

GRADUATE SCHOOL ADVANCED MATERIALS

This Graduate School is also under the leadership of IRIS member N. Koch, and with a total of nine IRIS members, the participation of IRIS Adlershof is again



very high. The *Graduate School Advanced Materials* was explicitly developed as a permanent university structure in response to demands for further strengthening of this research field and promotion of early-career researchers (see Chapter 5). It is therefore an essential contribution to the sustainability of the concept of IRIS Adlershof. The graduate school offers doctoral students structured support to attain excellent professional qualifications and competent assistance for their career development. Special emphasis is laid on the close integration of physics and chemistry, experiment and theory, as well as fundamental and application-related aspects. In May 2020, the first doctoral students were admitted.

ETN Ultra-high Charge Carrier Mobility to Elucidate Transport Mechanisms in Molecular Semiconductors (UHMob)



UHMob is a 48-months multi-site European Training Network aimed at enabling multidisciplinary

and cross-sectoral training and research in the field of organic electronics. IRIS Adlershof is involved in this project through its member N. Koch. UHMob gathers six universities, two research centers, and two companies in Europe, who have joined their forces to train 15 early-career researchers. The scientific objective of UHMob is to gain a fundamental understanding of charge transport mechanisms in molecular semiconductors. To this goal, bestperforming and well-characterized materials will be studied by a complementary set of methods, including field effect transistors, but also optical methods such as terahertz spectroscopy, and field-induced time-resolved microwave conductivity. UHMob will also explore the coupling of molecular semiconductors with the vacuum electromagnetic field, which is a radically new physical concept holding great promises to modulate optoelectronic properties of materials.

HI-ACCURACY

In April 2020, the ambitious EC Horizon 2020 funded project *High-ACCuracy*



printed electronics down to μm size, for Organic Large Area Electronics (OLAE) Thin Film Transistor (TFT) and Display Applications started with the participation of the Hybrid Devices group of E. List-Kratochvil and the coordination of the Austrian non-profit research institute Joanneum Research Forschungsgesellschaft mbH. In a joint approach, 11 project partners from six European countries are developing new printable materials and innovative additive fabrication processes to create next-generation display technologies. Materials such as quantum dots, novel organic semiconductors, and conductive inks that can be produced at low cost with minimal environmental impact are being developed. The three-year project is focused on producing a small-scale 'proof of concept' display screen. But it is anticipated that longer-term applications of the technology will be on larger, high-resolution displays for use in venues including transport hubs, civic centers, sports stadia, exhibition halls, and roadside information. At the other end of the scale it is expected that the displays will become the basis of personal devices including smart watches, phones, VR headsets.

3.2.3. RESEARCH AREA SPACE-TIME-MATTER

RTG 2575: RETHINKING QUANTUM FIELD THEORY



Particularly remarkable is the approval of the Research Training Group 2575 Rethinking Quantum Field

Theory in early 2020 with IRIS Adlershof's member J. Plefka as spokesperson. The RTG is a joint project of the Department of Physics at HU, DESY, and the Max Planck Institute for Gravitational Physics and is being funded by the German Research Foundation. The successful acquisition not only provides important impulses in the promotion of IRIS earlycareer researchers (see Chapter 5), it also strengthens the connection to IRIS Adlershof's important cooperation partners. As the young researchers work on pressing theoretical questions and key innovations in quantum field theory and theoretical particle physics that go beyond established methods, the RTG 2575 furthermore significantly advances research at IRIS Adlershof in mathematical physics. Participating IRIS members are V. Forini, O. Hohm, D. Kreimer, J. Plefka, and M. Staudacher.

ITN SAGEX – Scattering Amplitudes: From Geometry to Experiment



Among the remarkable third-party funded projects that launched during the reporting period and in which IRIS Adlershof's members

actively participate is furthermore the Innovative Training Network SAGEX. SAGEX started in September 2018 and is being funded by the European Union to train the next generation of world-leading scientists in the field of scattering amplitudes. At HU, two Ph.D. positions are funded for this purpose, one in the research group Mathematical Physics of Space, Time and Matter of IRIS member M. Staudacher and one in the research group Quantum Field and String Theory of IRIS member J. Plefka.

Kolleg Mathematik Physik Berlin



The Kolleg Mathematik Physik Berlin (KMPB) was established in 2015 as an interdisciplinary center at Humboldt-Universität zu Berlin and it was successfully extended twice during the reporting period. The KMPB is headed by D. Kreimer, who is a member of IRIS Adlershof. Other IRIS members involved in the KMPB are J. Plefka, M. Staudacher, O. Hohm, and V. Forini as well as N. Furey, who is a Freigeist Fellow at IRIS Adlershof. The community of *KMPB* research groups shares a mutual interest in mathematics and physics. Quantum field theory is their unifying theme, which connects to algebraic geometry, number theory, and differential geometry in mathematics, as well as to research in particle physics, gravitation, and string theory in physics. A highlight of *KMPB* activities is its international schools and workshops as for instance *Higgs Bundles, K3 surfaces and Moduli* (Berlin July 2017), *Local Quantum Field Theory* (Les Houches, France June 2018), and *From Classical Gravity to Quantum Amplitudes and Back* (Berlin November 2019).

3.2.4. Extension of Research Areas

As agreed with the university leadership, IRIS Adlershof should expand its existing research areas and establish new ones. IRIS Adlershof accepted this challenge and has taken the following measures:

COOPERATION WITH CULTURAL SCIENCES

For some years now, IRIS Adlershof has been devoting itself to new, cross-disciplinary perspectives with the EXC 1027 *Image Knowledge Gestaltung* and its successor EXC 2025 *Matters of Activity. Image – Space – Material*, which go beyond the two research areas Hybrid Systems for Optics and Electronics and Mathematical Physics of Space-Time-Matter, and at the same time link them. The EXC 2025 aims to create a basis for a new culture of materials. The central vision of the cluster is to



The interactive CUBE OF PHYSICS in the Department of Physics

rediscover the analog in the activity of images, spaces, and materials in the age of the digital. Biology and technology, mind and material, nature and culture intertwine in a new way. In this context, the interdisciplinary research and development of sustainable practices and structures is a central concern in areas such as architecture and soft robotics, textiles, materials and digital filters, and surgical cutting techniques. The cluster focuses on a new role of design, which is emerging in the context of growing diversity and the continuous development of materials and visualization forms in all disciplines.

From IRIS Adlershof J. P. Rabe und M. Staudacher are involved as principal investigators in three of altogether six different cluster-subprojects and work there closely together with scientists from many different disciplines such as architecture, art history, psychology, neuroscience, and cultural science. A particular project is the *Cube of Physics* and its recent extension, the *Hypercube of Physics*, together with C. Kassung from Cultural Sciences and several early-career researchers

BIG DATA

IRIS Adlershof has taken first steps towards establishing a new field of research, *Big Data*, at the interface of physics, mathematics, computer science, chemistry, and materials science. Innovative management of big data in computer-aided materials science is one of the main research areas of IRIS member C. Draxl. In recent years, Draxl and M. Scheffler from FHI in close cooperation, have built up the *Novel Materials Discovery Laboratory (NOMAD Lab)*, the world's largest database of material properties, which now contains 100 million calculations. Designed as a FAIR



The NOMAD General Structure

(Findable, Accessible, Interoperable, and Re-purposable) infrastructure, the *NOMAD Lab* enables the productive handling of scientific data and is thus, together with the use of Artificial Intelligence, essential for the development of future technologies. As part of the *NOMAD* Center of Excellence, which was renewed for a second funding period in 2020, Draxl and Scheffler are also developing computational materials science into new applications and preparing it for the next generation of high-performance computers (exascale computers). The CRC 1404 FONDA – Foundations of Workflows for Large-Scale Scientific Data Analysis, approved by the German Research Foundation in July 2020, also represents a further development of IRIS Adlershof in the direction of *Big Data*. In CRC 1404, an interdisciplinary group of PIs from computer science, material science, geosciences, and the life sciences investigates methods for increasing productivity in the development, execution, and main-tenance of Data Analysis Workflows for large scientific data sets. The long-term goal is to develop methods and tools that achieve substantial reductions in development time and development cost of DAWs. Spokesperson of the CRC is U. Leser from HU's Computer Science Department. Participating IRIS members are C. Draxl, C.T. Koch, and A. Reinefeld.

QUANTUM TECHNOLOGY

Furthermore, IRIS Adlershof expanded its spectrum towards a new field of research in *Quantum Technology*. The foundation for this was laid in the previous reporting period through IRIS founding member O. Benson and S. Ramelow, who has been with IRIS Adlershof since 2016, and who recently published a highly recognized article in Science Advances, describing the first infrared based microscope with quantum light. In 2018, this undertaking was further advanced by the granting and participation of Benson's and Ramelow's working groups in the joint project *Quantum Link Expansion* (*Q.Link.X*) that is being funded by the Federal Ministry of Education and Research. In *Q.Link.X* researchers explore the key technology of quantum repeaters. Since 24 partners from research institutions from universities to industrial laboratories are driving *Q.Link.X* together, this project strengthens the national standing of IRIS Adlershof and the HU on the scientific landscape. The admission of ERC Grant Holder T. Schröder as an IRIS member in 2019 and of M. Krutzik as junior member in 2021, are also steps towards establishing the new research field *Quantum Technology*.

CATALYSIS RESEARCH

Catalysis Laboratory

Catalysts are the key to many technologies and processes needed to build a climate-neutral economy. A

hotspot for catalysis research has been developing in Berlin's research landscape for some time. As part of the Excellence Strategy, new clusters such as *UniSysCat* have been created in which established research institutes bundle their activities and the chemical industry is involved through the

BASCat laboratory. An important field of research is the production of *green* hydrogen: in order to produce hydrogen and synthetic fuels in a climate-neutral way using renewable energies, innovative catalysts are needed. The recently launched Berlin-based *CatLab* project, which is funded as part of the federal Hydrogen Strategy, is pursuing completely new approaches based on thin-film technologies that promise real leaps in innovation.

To further promote catalysis research in Berlin, HU and HZB have now signed a cooperation agreement. Part of the laboratories in the new IRIS Research Building is additionally equipped for the development and investigation of heterogeneous catalyst systems. To study catalysts in action, electron microscopes have been set up in the basement. In addition, *in-operando* investigation methods such as X-ray diffraction, photoelectron, Raman, and UV-vis spectroscopy will be used, which will be completed by the high-end analysis options of the neighboring synchrotron radiation source BESSY II of the HZB. Close cooperation is also planned in the field of thin-film technology, using additive manufacturing processes and nanostructuring and synthesis methods.

3.2.5. Gender Equality and Family Friendliness

IRIS Adlershof sees itself as a place of diversity, plurality of opinion, mutual appreciation, and respect. Therefore, it is attaching great importance to the provision of equal opportunities. The respective key measures are outlined in the following.

Since female scientists are unfortunately still underrepresented in some disciplines of natural sciences, namely in physics, IRIS Adlershof provided particular administrative and financial support to its female scientists during the reporting period. The promising Ph.D. students B. Rezania, F. Davidson-Marquis, and A. Manoharan were actively supported in taking the next step in their academic careers through interim financing and scholarships, that enabled them to begin, as well as successfully complete, their doctorates and to publish their results. A. Valencia was partially funded a post-doctoral position and provided work opportunities with IRIS funding so that she could continue her research in the IRIS research area *Hybrid Systems*.

The IRIS flagship project CRC 951 *HIOS* (spokesperson N. Koch, IRIS Adlershof) is also strongly committed to gender equality and family friendliness. E.g., it partners with WiNS (Women in Natural Science) Adlershof and covers the

costs of workshops, job trainings, coaching, and mentoring for its female scientists. The WiNS Adlershof program aims at encouraging young women to pursue a scientific career. In 2019, CRC 951 and IRIS Adlershof member C. Cocchi coorganized a WiNS Summer School that introduced female students and doctoral students on the topics of spectroscopy and light-matter interactions. IRIS Adlershof and HIOS funded it proportionally. HIOS also organizes once per funding period a scientifically oriented HIOS Gender Equality Workshop for their members. In collaboration with Club Lise mentoring, HIOS has established scientific visiting programs for female pupils such as Forscherinnen-Tag and Schülerinnen on Tour. These programs include interactive scientific presentations, demonstration experiments, and hands-on experience with authentic experimental equipment. Furthermore, HIOS offers child care support to its members through cooperation with daycare centers with extended opening hours and the Kidsmobile, a mobile childcare service that can step in at short notice. Moreover, a family room that enables parents to combine work and supervision of children and, if necessary, also offers a protected space for paernts, has been set up in the IRIS Research Building.

4. Cooperation and International Visibility

As stated in the agreement between HU and IRIS Adlershof, the increase of the institute's international visibility and the profiling of the Campus Adlershof as a place for internationally recognized top-level research were (and still are) two of IRIS Adlershof's central goals. Therefore, IRIS Adlershof initiated new and intensified existing fruitful cooperation with international partner institutions worldwide during the reporting period.

INTERNATIONAL COOPERATIONS:

Chiba U	Chiba University, Japan
ETH Zürich	Swiss Federal Institute of Tech-
	nology Zurich, Switzerland
IOPCAS	Institute of Physics of the Chinese
	Academy of Sciences, China
NUS	National University of Singapore
Princeton U	Princeton University, USA



FU Berlin	Freie Universität Berlin
TU Berlin	Technische Universität Berlin
U Potsdam	Universität Potsdam

INDUSTRIAL PARTNERS:

Inuru	Inuru GmbH
Oreltech	OrelTech GmbH
xolo	Xolo GmbH

COOPERATION NETWORKS:

- INAM Innovation Network for Advanced Materials
- FAIR-DI FAIR Data Infrastructure for Physics, Chemistry, Materials Science, and Astronomy e.V.
- Cooperations with Non-University Research Institutions:
- AEI Max Planck Institute for Gravitational Physics (Albert-Einstein-Institute)

BAM	Federal Institute for Materials Research and Testing (BAM)
Charité	Charité-Universitätsmedizin Berlin
FBH	Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik
FHI	Fritz-Haber-Institut der Max-Planck-Gesell- schaft
нні	Fraunhofer Heinrich Hertz Institut
HZB	Helmholtz Zentrum Berlin
IAP	Fraunhofer Institute for Applied Polymer Re- search
IKZ	Leibniz Institute for Crystal Growth
MBI	Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy
MPI-KG	Max Planck Institute of Colloids and Interfaces
MPI-P	Max-Planck-Institute for Polymer Research
PDI	Paul-Drude-Institut für Festkörperelektronik
WIAS	Weierstraß-Institut für Angewandte Analysis und Stochastik
ZIB	Konrad-Zuse-Zentrum für Informationstechnik Berlin

COOPERATIONS



IRIS Adlershof promotes intra-university collaboration with a strong research focus and thus plays a decisive role in profile-building at

the university, namely, in the natural sciences. As an interdisciplinary institute, IRIS Adlershof is transversally positioned to Humboldt-Universität's disciplinary natural science departments of Chemistry, Computer Sciences, Mathematics, and Physics as well as the Department of Cultural Sciences. The interdisciplinarity is fostered through the cooperation with both the Faculty of Natural Sciences and the Central Institute Hermann von Helmholtz-Centre for Cultural Techniques.

Among the most important university cooperation partners of IRIS Adlershof are primarily the Berlin universities TU, FU and Charité, which form the BUA, as well as the University of Potsdam, which is in the immediate vicinity of Berlin. Cooperation with non-university research institutions in the Berlin Brandenburg region (BR 50) is of particular importance to IRIS Adlershof. In this respect, among others, the HZB with its electron storage ring for synchrotron radiation BESSY II as well as the FHI, the MBI, the WIAS and the ZIB are particularly noteworthy.

JOINT LAB GENFAB

A further significant achievement is the establishment of the Joint Lab Generative manufacturing processes for hybrid components (GenFab) by IRIS Adlershof and HZB. In GenFab, the group of E. List-Kratochvil closely collaborates with the Young Investigator Group Hybrid Materials Formation and Scaling led by E. Unger from HZB, and the HySPRINT perovskite lab. Their long-term collaboration focuses on the generative manufacturing processes for hybrid components. The emphasis is not only on basic research but also on advancing the industrial application through accompanying process development. The goal is to develop large-scale (opto)electronic devices, printed solar cells, and components fabricated by printing and solution-based methods from hybrid materials: from transparent conductive electrodes to memory devices, transistors, light-emitting diodes, solar cells, and sensor applications. For IRIS scientists, the collaboration is significant not only because of the acquisition of important cooperation partners. The partnership also makes it possible to build bridges from academia to industry. To enforce the synergy between the research groups, IRIS Adlershof established a new jointly used lab space for *GenFab*



based in the new IRIS Research Building.

Cooperation with Industrial Partners

IRIS Adlershof's collaboration with partners from industry has expanded enormously in the research area *Hybrid Materials* during the reporting period. The very good cooperation with the start-up companies INURU and Oreltech is the result of IRIS Adlershof's involvement in *INAM*. INURU prints OLED technology, lets packaging labels and magazine covers light up, and participates in the development of innovative battery systems. OrelTech develops conductive inks based on ionic precious metals. This enables transparent conductor paths to be incorporated into touch displays, OLEDs, or flexible solar cells in inkjet printing processes and circuits to be printed on two- and three-dimensional objects. Scientists at IRIS Adlershof benefit from the concrete applications of the start-ups because they bring their research in the field of hybrid systems into direct relation to practice-relevant issues. On the other hand, the cooperation is a huge



opportunity for the startups because they can test and examine their materials with the help of the excellent

IRIS Adlershof infrastructure.

The Berlin-Adlershof based start-up xolo GmbH was founded by IRIS member S. Hecht together with the physicist M. Regehly, a former HU physics' graduate, and the former CEO of Humboldt Innovation GmbH. D. Radzinski. Xolo has developed a disruptive new additive manufacturing technology and recently started to commercialize the first volumetric 3D printer (XUBE). Their invention, called xolography, is based on Hecht's specialty: photoswitchable molecules, which only at the crossing (x) of light rays of two different colors allow precise curing of the photopolymer resin in the entire volume (holos). In contrast to conventional 3D printing, in which objects are created layer by layer, the advantages of xolography are the continuous printing process leading to homogeneous materials with smooth surfaces and the significantly higher build speed without compromising for resolution. Moreover, fully assembled multicomponent systems can be fabricated in just one step.

INTERNATIONAL COLLABORATION WITH PROFILE PARTNERS

Fostering long-term and intensive cooperation with HU's profile partners, the National University of Singapore and Princeton University in the research area *Novel (Opto-) Electronic Materials* is also of great importance for IRIS Adlershof.

An immensely fruitful collaboration between Andrivo Rusidy from NUS and IRIS member C. Draxl is based on their common interest in solar cell materials, investigating their interaction with radiation from two different perspectives, namely, experiment on the NUS side and *ab ignitio* theory on the HU side. Concerning kersterites, a puzzling seeming discrepancy between different X-ray absorption measurements (K- edge and L2,3-edge, performed on different samples) and theoretical results could be solved by performing both probes (K- and L-edge) on a dedicated new sample at NUS. In-depth analysis based on many-body theory calculations finally revealed the different nature of the used samples, being either disordered or copper-poor. Another focus is 2D hybrid perovskites, where common investigations are dedicated to exploring the effect of spin-orbit coupling on the excitation spectra. The joint research effort with researchers from Princeton University was established to study the fundamental chemical, electronic, and photonic interactions in novel optoelectronic materials and their combinations, and at developing new device types and architectures, including addressing manufacturing issues. To further strengthen this important international cooperation, IRIS Adlershof supported the scientifically highly *acclaimed Gordon Research Conference: Electronic Processes in Organic Materials* financially in July 2018. Amongst the invited speakers of the conference were the IRIS members N. Koch and C. Draxl.

Partnership with the Chinese Academy of Sciences

Particularly noteworthy is the newly established scientific cooperation between IRIS Adlershof and the Institute of Physics (IOP) of the Chinese Academy of Sciences (CAS). The partnership began with joint workshops and delegation visits in 2019. The focus of interest was priority subjects at

both institutes, including 2D- and nano-materials, soft matter, hybrid electronic devices, photoemission, synchrotron research, and quantum information. In September 2020, a Memorandum of Understanding was signed.



The most recent success of this international cooperation between the IOP and IRIS Adlershof is a joint postdoctoral program. The prestigious two-year research fellowships are intended for exceptional early-career researchers, in preparation for an independent career in research at the frontier of condensed matter physics, quantum materials, or device physics. Successful candidates will spend one year at the IOP Zhongcuancun Beijing Campus and one year in Berlin at the Campus Adlershof in the research groups of their choice. The fellows can visit and interact with associated partners of IRIS Adlershof, including the Max Born Institute, the HZB and its Electron Storage Ring BESSY II, the FU Berlin, and the IKZ. They will be financially supported by up to 4,500 EUR/month, the first round of applications began in early 2021.

Welcoming Guest Researchers

Hosting guest researchers is also very important for the expansion of IRIS Adlershof's international relations, as they provide an important impetus for research conducted at the institute. During the reporting period, IRIS Adlershof not only hosted guest scientists but also laid the foundation for successful future cooperation:

J.-L. Bredas, professor and department head for Chemistry and Biochemistry at the University of Arizona - Tucson, was

awarded the Humboldt Research Award in 2019. Bredas is internationally recognized for his groundbreaking contributions in the field of organic semiconductors. The continuous impact of his research on the field is reflected by numerous awards and honors. He has been ranked among the 100 top chemists in the world, the 100 top materials scientists in the period 2000 – 2010, and the most highly cited researchers in 2018. Bredas will visit IRIS Adlershof and collaborate with the groups of the IRIS members C. Draxl and N. Koch to expand joint work in the area of hybrid organic-inorganic interfaces.

Carlos-Andres Palma, professor at the Institute of Physics / Chinese Academy of Sciences, has been researching at IRIS

Adlershof as part of his fellowship granted by the Alexander von Humboldt Foundation. Together with the groups of IRIS Director J. P. Rabe and Deputy Director N. Koch, Palma explores nanographene materials and their phonon properties in the project *Low-dimensional carbon sp3 materials at welldefined interfaces*. He contributes with his expertise in ultrahigh-vacuum variable



Carlos Andres Palma
temperature and low-temperature atomic force microscopy (AFM), and complementary surface analytics.

In September 2020 the mathematical physicist Nichol Furey (U Cambridge), joined IRIS Adlershof as a Freigeist fellow of the Volkswagen Foundation, to study a special number system, the octaves. She would like to prove that the behavior of elementary particles can be predicted using this system. Her project *In-depth Study into the Algebraic Structure of Elementary Particle Physics* explores the question of whether there is a mathematical logic behind the inner processes of elementary particle physics. She collaborates closely with the IRIS groups of J. Plefka, M. Staudacher, and D. Kreimer.



Nichol Furey © Jan Zappner

International Symposium $F\pi_{14}$

The common objective of IRIS Adlershof and HU to increase the international visibility of the institute and the campus was also implemented on site. In June



2019, IRIS Adlershof jointly organized the 14th International Symposium of Functional π-Electron Systems together with the HZB in Adlershof. The scientific program was co-organized by the IRIS members S. Hecht and N.

Koch. The F π symposia are among the most important and influential international symposia in the diverse areas of π -electron systems research and have been held only three times in Europa so far. Therefore, this was a further significant impulse for the international recognition of IRIS Adlershof and the importance of the Science and Technology Park Adlershof as a place for excellent research. A total of over 500 guests were welcomed and important contacts were made for follow-up discussions

5. **PROMOTION OF EARLY-CAREER RESEARCHERS**

Following the recommendation of the expert commission (previous evaluation of IRIS) and with the aim of continuous further improvement, IRIS Adlershof has expressively expanded its measures for the promotion of early-career researchers.

EARLY-CAREER PROMOTION

During the reporting period, all members of IRIS Adlershof were teaching classes in the study programs of their primary disciplinary departments, and gave additional lectures to convey the IRIS research. As a matter of course, they directly supported early-career researchers in their work towards bachelor, master, and doctoral theses. Furthermore, as stated in the agreement with HU, IRIS Adlershof followed the request to increase its commitment to the existing master programs *Polymer Science* and *Optical Science*. HU offers these programs together with university and non-university cooperation partners from the Berlin/Brandenburg region. These measures were intended to attract the interest of master and doctoral students in the science done in IRIS Adlershof and thus to integrate them into IRIS research at an earlier stage.

Implementation of New Doctoral Programs

The promotion of early-career researchers at IRIS Adlershof was enhanced by the implementation of one new doctoral program in each IRIS research area – the *Graduate School Advanced Materials* in the research area *Hybrid Systems for Optics and Electronics* and the RTG 2575 in the research area *Mathematical Physics of Space–Time–Matter.* Both programs have been in operation since spring 2020 and offer early-career researchers excellent career-building opportunities, both in scientific and transferable skills. The EU training programs, like SAGEX, in which IRIS Adlershof is involved through its members are additional strong component in the promotion of early-career researchers. Through these measures, IRIS Adlershof commits to excellence in graduate education and to support early-career researchers Adlershof in professional career development.

Administrative and Financial Support

IRIS Adlershof also offers administrative and financial support to its early-career researchers. As a service provider in

science management, IRIS Adlershof assists, for example, in setting up their working groups or in organizing scientific events. Within the institutional scope of available funds, IRIS Adlershof awarded fellowships to early-career researchers and issued a corresponding guideline in May 2020. The fellowship is intended to enable the re-cipient to fully dedicate to the implementation or completion of their research project, or to apply for own third-party funds, all aligned with the IRIS research program. During the reporting period, several high-potentials were supported in taking the next step in their academic careers through interim financing.

Events Aimed at Early-Career Researchers

The IRIS Symposium in 2019 was also aimed at promoting the careers of researchers at an early stage. To increase the number of presentations by early-career researchers within the limited time of a symposium, the format was expanded to feature a poster session with a competition. The winner Dr. Benedikt Hass received a voucher for a travel allowance for participation in a conference.

In early 2020, IRIS Adlershof had to stop events with presence *in persona* due to the pandemic. Selected events, suitable for online formats, were yet carried out.

ACHIEVEMENTS OF IRIS EARLY-CAREER RESEARCHERS

In April 2020, IRIS Adlershof junior group leader Michael J. Bojdys became one of the first two ERC Proof of Concept grantees in Berlin since the grant was established in 2018. Proof of Concept (PoC) grants are exclusively awarded to researchers who already hold an ERC Grant and wish to move the output of their research towards the initial steps of precommercialization. In the course of his ERC PoC Grant *Ultrahigh energy storage Li-anode materials (LiAnMAT)* Bojdys will develop, together with VARTA Micro Innovation GmbH and the Adlershof start-up INURU GmbH, Li anode materials for

high capacity applications. The first promising results are part of a patent application of HU and the start-up incubator Humboldt Innovation GmbH.

In the light of these remarkable achievements, IRIS Adlershof continues to regard the support of earlycareer researchers as toppriority.



Michael J. Bojdys

6. SCIENTIFIC HIGHLIGHTS

OPTICAL COHERENCE TOMOGRAPHY (OCT) ON HIGHLY SCATTERING AND POROUS MATERIALS

Aron Vanselow, a young researcher at IRIS Adlershof, shows an attractive approach that makes it easier to perform optical coherence tomography (OCT) on highly scattering and porous materials. It specifically demonstrates that entangled photons can be used to improve the penetration depth of (OCT) in highly scattering materials. The method represents a way to perform OCT with mid-infrared wavelengths and could be useful for non-destructive testing and analysis of materials such as ceramics and paint samples.

OCT is a non-destructive imaging method that provides detailed 3D images of subsurface structures. OCT is typically performed using visible or near-infrared wavelengths because light sources and detectors for these wavelengths are readily available. However, these wavelengths don't penetrate very deeply into highly scattering or very porous materials. Aron Vanselow and colleagues from Humboldt-Universität zu Berlin in Germany, together with collaborators at the Research Center for Non-Destructive Testing GmbH in Austria, now demonstrate a proof-of-concept experiment for mid-infrared OCT based on ultra-broadband entangled photon pairs. They show that this approach can produce high quality 2D and 3D images of highly scattering samples using a relatively compact, straightforward optical setup.

Researchers used entangled photons to increase the penetration depth of OCT for scattering materials. They demonstrated the technique by analyzing two alumina ceramic stacks containing laser-milled microchannels. The midinfrared illumination allowed the researchers to capture depth information and to create a full 3D reconstruction of the channel structures (pictured).

"Our method eliminates the need for broadband mid-infrared sources or detectors, which have made it challenging to

6. Scientific Highlights



develop practical OCT systems that work at these wavelengths," said Vanselow. "It represents one of the first realworld applications in which entangled photons are competitive with conventional technology."

The technique could be useful for many applications including analyzing the complex paint layers used on airplanes and cars or monitoring the coatings used on pharmaceuticals. It can also provide detailed 3D images that would be useful for art conservation. For this technique, the researchers developed and patented a nonlinear crystal that creates broadband photon pairs with very different wavelengths. One of the photons has a wavelength that can be easily detected with standard equipment while the other photon is in the mid-infrared range, making it difficult to detect. When the hard-to-detect photons illuminate a sample, they change the signal in a way that can be measured using only the easy-todetect photons.

"Our technique makes it easy to acquire useful measurements at what is a traditionally hard-to-handle wavelength range due to technology challenges," said Sven Ramelow, who conceived and guided the research. "Moreover, the lasers and optics we used are not complex and are also more compact, robust and cost-effective than those used in current mid-infrared OCT systems."

To demonstrate the technique, the researchers first confirmed that the performance of their optical setup matched theoretical predictions. They found that they could use six orders of magnitude less light to achieve the same signal-tonoise ratio as the few conventional mid-infrared OCT systems that have been recently developed. "We were positively surprised that we did not see any noise in the measurements beyond the intrinsic quantum noise of the light itself," said Ramelow. "This also explained why we can achieve a good signal-to-noise ratio with so little light."

The researchers tested their setup on a range of real-world samples, including highly scattering paint samples. They also analyzed two 900-micron thick alumina ceramic stacks containing laser-milled microchannels. The mid-infrared illumination allowed the researchers to capture depth information and to create a full 3D reconstruction of the channel structures. The pores in alumina ceramics make this material useful for drug testing and DNA detection but also highly scattering at the wavelengths traditionally used for OCT.

The researchers have already begun to engage with partners from industry and other research institutes to develop a compact OCT sensor head and full system for a pilot commercial application.

Frequency-domain optical coherence tomography with undetected mid-infrared photons

A. Vanselow, P. Kaufmann, I. Zorin, B. Heise, H. M. Chrzanowski, S. Ramelow *Optica* 2020, 7(12), 1729. doi: 10.1364/OPTICA.400128

XOLOGRAPHY AS NEW VOLUMETRIC 3D PRINTING METHOD

It looks like science fiction but in fact could be the future of 3D printing: A blue slice of light wanders through a liquid, while light projections emerge through the window of a glass vessel. Resembling the replicator of the Star Trek spaceships, the desired object materializes. What used to take hours soon floats in the liquid in the vessel, is then removed, and cured under UV light.

The underlying process – xolography – was developed by a team led by chemist Stefan Hecht from IRIS Adlershof, phys-

icist Martin Regehly, and the founder Dirk Radzinski in the startup company xolo GmbH in Berlin Adlershof over the past two years. For the first time, they now describe their unique method in the renowned journal Nature.

Their invention is based on Hecht's specialty: photoswitchable molecules, which only at the intersection (xolography) of light rays of two different colors allow precise curing of the starting material in the entire volume (holos). In combination with a new printing process (xolography) based on a



laser-generated light sheet and projected cross-sectional images, the desired objects are generated from virtual 3D models.

In contrast to conventional 3D printing, in which the objects are created layer by layer, the advantages of xolography are the significantly higher build speed that is due to the higher efficiency of combining two linear one-photon processes as opposed to non-linear two-photon stereolithography. The faster build speed does not compromise for resolution and thus smooth surfaces can be created. Moreover, fully assembled multicomponent systems can be fabricated in just one step.

Hecht is amazed "to see how fast this has been moving from an idea to xolo's first prototype printer, the XUBE. Working in a highly interdisciplinary team including chemists, physicists, materials scientists, and software developers with a clear focus and dedication, we have been able to develop xolography as a powerful new method." He is excited about the many opportunities ahead: "The beauty is our method's versatility as we can print hard as well as soft objects. This should have major implications for the future manufacturing of optical, (micro)fluidic, and biomedical devices."

Xolography for linear volumetric 3D printing

M. Regehly, Y. Garmshausen, M. Reuter, N.F. König, E. Israel, D.P. Kelly, C.-Y. Chou, K. Koch, B. Asfari, and S. Hecht, *Nature*, 2020, 588(7839), 620. doi: 10.1038/s41586-020-3029

Molecular telegraphy: Sending and receiving individual molecules precisely

The concept of throwing and catching a ball is familiar to everyone and works well in the macroscopic world. But could this be done in the nanoworld using individual molecules instead? And if one could transfer molecules precisely back and forth between two distant places, how fast would they be? An international team involving Stefan Hecht, who is a member of IRIS Adlershof, found some spectacular answers to these questions and the results of their study have been published as the cover story a recent issue of Science magazine.

"Through the targeted movement of individual molecules, we can gain insight into fundamental physical and chemical processes that are important for molecular dynamics - for example during chemical reactions or in catalysis," explains Leonhard Grill from the University of Graz, who led the team. For the study, the scientists brought organic molecules about two nanometers long on a silver surface with the fine metal tip of a scanning tunneling microscope in a special orientation, in which they are still extremely mobile, even at -



266 °C. "We were able to show that, despite the very flat surface, the molecules move along a single row of atoms, *i.e.* only in one direction," the researcher describes.

If an electric field is switched on, individual molecules can be moved perfectly along a straight line by electrostatic forces, as if the molecule would be on rails. As a result, the molecules can – depending on the direction of the field – be sent and received in a targeted manner by the forces of repulsion and attraction, respectively. The uncovered phenomenon operates over relatively long distances of 150 nanometers and at the same time with extremely high precision of 0.01 nanometers. The researchers were able to measure the time it took an individual molecule to be transferred and thus could determine the speed of an individual molecule directly. At these low temperatures, the molecule moved at 0.1 mm per second over the silver surface. These studies provide completely new possibilities for the investigation of molecular energies during movement and more importantly during chemical reactions. At Oak Ridge National Laboratory, the researchers were able to carry out a unique transmitter-receiver experiment. Specifically, two separate scanning tunnel microscope tips were first appropriately positioned. Upon switching the "transmitter tip" from attractive to repulsive mode, the molecule moved precisely to the location of the "receiver tip". This allowed to characterize the molecular motion and deduce the speed. But moreover this experiments illustrates the great potential for information transfer since all information stored in the molecule can be transferred with exquisite spatial precision."

Control of long-distance motion of single molecules on a surface

D. Civita, M. Kolmer, G. J. Simpson, A.-P. Li, S. Hecht, and L. Grill

Science, 2020, 370(6519), 957. doi: 10.1126/science.abd0696

Implementation of Flexible Embedded Nanowire Electrodes in OLEDs

Researchers in the HySPRINT joint lab Generative manufacturing processes for hybrid components (GenFab) of Humboldt-Universität zu Berlin (HU) and Helmholtz-Zentrum Berlin (HZB) have developed together with the Austrian Institute of Technology (AIT) a method to produce flexible transparent electrodes based on silver nanowires. Specifically, the nanowires are spray coated and embedded within a polymer resin on top of polyethylene terephthalate (PET) substrate. Not only are the electrodes fabricated using solution-based approaches, but compared with the widely used indium tin oxide (ITO), the electrodes show higher stability in mechanical bending tests. "Since the spray coating approach in this work can be upscaled to larger areas", says Dr. Felix Hermerschmidt, senior researcher in the joint lab of HU and HZB, "this mechanical stability can be translated to an industrial process."

The researchers fabricated organic light-emitting diodes employing the developed ITO-free nanowire electrodes. These show considerably higher luminance values at the same efficacy compared to their ITO-based counterparts. As Dr. Theodoros Dimopoulos, senior scientist at AIT, points out,



"Replacing ITO in optoelectronic devices is a key area of research and this work shows the possibilities of doing so without loss in performance."

GenFab, led by IRIS Adlershof member Prof. List-Kratochvil, is moving in laboratory rooms in the new IRIS-research building for further development.

Implementation of Flexible Embedded Nanowire Electrodes in Organic Light-Emitting Diodes

L. Kinner, F. Hermerschmidt, T. Dimopoulos, and E.J.W. List-Kratochvil

Physica Status Solidi Rapid Res. Lett., 2020, 14(11), 2000305. doi: 10.1002/pssr.202000305

IS QUANTUM LIGHT MICROSCOPY THE FUTURE OF BIO-MEDICINE?

Researchers from Humboldt-Universität zu Berlin and the Experimental and Clinical Research Center (ECRC) built the first infrared based microscope with quantum light. By deliberately entangling the photons, they succeeded in imaging tissue samples with previously invisible bio-features.

The researcher team from Humboldt-Universität zu Berlin and the Experimental and Clinical Research Center (ECRC), a joined institution from Charité – Universitätsmedizin Berlin and Max Delbruck Center for Molecular Medicine in the Helmholtz Association, is featured on the cover of 'Science Advances' with their new experiment. For the first time they successfully used entangled light (photons) for microscope images. This very surprising method for quantum imaging with undetected photons was only discovered in 2014 in the



Quantum microscopy of a mouse heart. Entangled photons allow for the making of a high-resolution mid-IR image, using a visible light (CMOS) camera and ultralow illumination intensities. In the picture, absorption (left) and phase information (right) from a region in a mouse heart. The yellow scale bar corresponds to 0.1 mm which is about the width of a human hair. group of the famous quantum physicist Anton Zeilinger in Vienna. The first images show tissue samples from a mouse heart.

The team uses entangled photons to image a bio-sample probed by 'invisible' light without ever looking at that light. The researchers only use a normal laser and commercial CMOS camera. This makes their MIR microscopy technique not only robust, fast and low noise, but also cost-effective making it highly promising for real-world applications. This use of quantum light could support the field of biomedical microscopy in the future.

Current camera detection is unequivocally dominated by silicon based technologies. There are billions of CCD (charge coupled device) and CMOS (complementary metal oxide semiconductor) sensors in digital cameras, mobile phones or autonomous vehicles. These convert light (photons) into electrical signals (electrons). But like our human eyes, these devices cannot see the important mid-IR range. This wavelength range is very important for biological science, containing valuable bio-chemical information that allows researchers to tell different biomolecules apart. The few camera technologies that exist at these crucial wavelengths are very expensive, noisy and subject to export restrictions. That is why the huge potential mid-IR light has for the life sciences so far remained unfulfilled. But researchers have proposed a new solution: "Using a really counterintuitive imaging technique with quantum-entangled photons allows us to measure the influence of a sample on a mid-IR light beam, without requiring any detection of this light" explains Inna Kviatkovsky, the lead author of the study.

There is also no conversion or so-called 'ghost-imaging' involved, but the technique relies on a subtle interference effect: first a pair of photons is generated by focusing a pump laser into a nonlinear crystal. This process can be engineered, such that one of the photons will be in the visible range and the other one in the MIR (invisible). The MIR photon probes the sample and is together with the visible photon and the laser sent back to the crystal. Here, quantum interference takes place - between the possibilities of the photon pair being generated on this first pass, and the possibility of not being generated on the first pass, but instead on the second pass through the crystal. Any disturbance, *i.e.* absorption caused by the sample, will now affect this interference and intriguingly this can be measured by only looking at the visible photons. Using the right optics one can build a mid-IR microscope based on this principle, which the team showed for the first time in their work.

"After a few challenges in the beginning, we were really surprised how well this works on an actual bio-sample." Kviatkovsky notes. "Also we shine only extremely low powers of mid-IR light on the samples, so low, that no camera technology could directly detect these images." While this is naturally only the first demonstration of this microscopy technique, the researchers are already developing an improved version of the technique. The researchers envisage a mid-IR microscope powered by quantum light that allows the rapid measurement of the detailed, localized absorption spectra for the whole sample. "If successful this could have a wide range of applications in label-free bio-imaging and we plan to investigate this with our collaboration partners from ECRC", Dr. Sven Ramelow, group leader at Humboldt-Universität zu Berlin, explains.

Microscopy with undetected photons in the mid-infrared

Inna Kviatkovsky, Helen M. Chrzanowski, Ellen G. Avery, Hendrik Bartolomaeus, and Sven Ramelow *Science Advances*, 2020, 6(42), eabd0264. doi: 10.1126/sciadv.abd0264

GRAPHENE AS A DETECTIVE TO UNRAVEL MOLECULAR SELF-ASSEMBLY

Researchers from Humboldt-Universität zu Berlin, the DWI – Leibniz Institute for Interactive Materials, and RWTH Aachen University (Germany), in collaboration with the University of Strasbourg & CNRS (France), have demonstrated that graphene devices can be used to monitor in real time the dynamics of molecular self-assembly at the solid/liquid interface. Their results have been published in Nature Communications.

Molecular self-assembly on surfaces is a powerful strategy to provide substrates with programmable properties. Understanding the dynamics of the self-assembly process is crucial to master surface functionalization. However, real-time monitoring of molecular self-assembly on a given substrate is complicated by the challenge to disentangle interfacial and bulk phenomena.

Cutting-edge scanning probe microscopy techniques, such as scanning tunneling microscopy (STM), have been used to monitor the dynamics of self-assembly at the solid/liquid interface, but thus far only in small populations of (less than 1,000) molecules and with a low time resolution (from 1 to 10 seconds). In the present study, the European research team led by Marco Gobbi and Paolo Samorì has shown that a transistor incorporating graphene – a two-dimensional (2D) material that is highly sensitive to changes in its environment – can be used as a highly sensitive detector to track the dynamics of molecular self-assembly at the graphene/solution interface.

A photoswitchable spiropyran molecule, equipped with an anchoring group and able to reversibly interconvert (switch) between two different forms (isomer) by light, was investigated. When a droplet of a solution of this compound is casted on graphene, the spiropyran isomer does not form any ordered adlayer on the surface. In strong contrast, upon ultraviolet (UV) irradiation, the molecules in solution switch to the planar merocyanine isomer that forms a highly ordered layer on the graphene surface. When the UV light is turned off, the molecules revert to their initial non-planar spiropyran form and the ordered adlayer desorbs. Importantly, the merocyanine monolayer induces a distinct change in the electrical conductance of graphene and hence it is possible to monitor the dynamics of its formation and desorption by simply recording the electrical current flowing through graphene over time.



A droplet of a solution containing a photochromic molecule is casted onto a graphene device. UV light is employed to induce photoisomerization, triggering the formation of an ordered assembly on graphene, which desorbs after UV light is turned off. The time evolution of the current flowing through the device allows monitoring the dynamics of formation and dissolution of the self-assembled adlayer.

This simple and robust platform based on a graphene device allows the real-time monitoring of the complex dynamic process of molecular self-assembly at the solid/liquid interface. The electrical detection, which is highly sensitive, ultra-fast, practical, reliable and non-invasive, provides insight into the dynamics of several billions of molecules covering large areas $(0.1 \times 0.1 \text{ mm}^2)$ with a high temporal resolution (100 ms). Furthermore, the ultra-high surface sensitivity of 6. Scientific Highlights

graphene permits to disentangle the dynamics of different processes occurring simultaneously at the solid/liquid interface and in the supernatant solution. This strategy holds a great potential for applications in (bio)chemical sensing and diagnostics.

Graphene transistors for real-time monitoring molecular self-assembly dynamics

M. Gobbi, A. Galanti, M.-A. Stoeckel, B. Zyska, S. Bonacchi, S. Hecht, and P. Samorì *Nat. Commun.*, 2020, 11(1), 4731. doi: 10.1038/s41467-020-18604-4

FIRST QUANTUM MEASUREMENT OF TEMPERATURE IN A LIVING ORGANISM

The exact measurement of temperature with highest spatial resolution in living organisms is of great importance in order to be able to investigate metabolic processes precisely. However, such a measurement was previously impossible due to the lack of precise and reliable nano thermometers or nano temperature probes. An international research team led by Prof. Oliver Benson, member of IRIS Adlershof, and Prof. Masazumi Fujiwara from Osaka City Universitity has now developed a quantum sensor that is only a few nanometers in size and has been able to measure temperature changes in a nematode after administration of a pharmacological substance. The results pave the way for diverse applications of the novel quantum sensors in biomedical research, *e.g.* for taking high-resolution thermal images.

In their experiment, the scientists used small diamonds with a diameter of a few 10 nanometers (1 nanometer = 1 millionth of a millimeter). These nanodiamonds contain luminous (fluorescent) quantum defects that can be observed under an optical microscope. With the help of radiated microwaves one can change the brightness of the luminous quantum defects. At a very specific microwave frequency, the defects appear a little darker. This so-called resonance frequency depends on the temperature. The researchers were now able to determine the shift in the resonance frequency very precisely and thus precisely determine the temperature change at the location of the nanodiamonds.



Scheme of the experiment: With the help of laser light (green), the characteristic microwave resonance line (in orange: microwave antenna) of nanodiamonds in a nematode (typical length 1 mm) can be recorded under a microscope. Since this depends on the temperature, a temperature change can be measured very precisely and locally. (©Masazumi Fujiwara, Osaka City University)

The nanodiamonds were inserted into a nematode (C. elegans). C. elegans is a very well understood model system and is examined in a large number of biophysical and biochemical experiments. By administering a certain pharmacological substance, the mitochondria, the "power stations" of the cells, could be stimulated to increased activity in individual cells of the worm. This then showed up as a slight local temperature increase of a few degrees.

The researchers were fascinated by the results of the experiment. "I never would have thought that the new methods of quantum technology would work so well even in living organisms," said Masazumi Fujiwara, professor at Osaka City University. "With these promising results, we are very confident that quantum sensing will establish in biochemistry and biomedicine. "adds Prof. Oliver Benson from Humboldt-Universität zu Berlin. The research teams are now working on further improving and automating their measuring method so that it can be easily integrated into standard microscopy setups.

Real-time nanodiamond thermometry probing in vivo thermogenic responses

M. Fujiwara, S. Sun, A. Dohms, Y. Nishimura, K. Suto, Y. Takezawa, K. Oshimi, L. Zhao, N. Sadzak, Y. Umehara, Y. Teki, N. Komatsu, O. Benson, Y. Shikano, and E. Kage-Nakadai,

Science Advances, 2020, 6(37), eaba9636. doi: 10.1126/sciadv.aba9636

Enwrapping of tubular J-aggregates of amphiphilic dyes for stabilization and further functionalization

The fabrication of functional units on mesoscopic length scales (nanometers to micrometers) in an aqueous environment by a self-assembling process is a fascinating but challenging task. It is essentially a biomimetic approach following design rules of living biological matter utilizing electrostatic and hydrophobic forces for the combination of a variety of materials. A peculiar form of such self-assembled structures is represented by tubular J-aggregates built from amphi-philic cyanine dye molecules. Those aggregates have attracted attention because of their similarity with natural light harvesting complexes. In particular, the dye 3,3'-bis(3sulfopropyl)-5,5',6,6'-tetra-chloro-1,1'-dioctylbenzimida-carbocyanine (C8S3) forms micrometer long double walled tubular aggregates with a uniform outer diameter of 13 ± 0.5 nm. These J-aggregates exhibit strong exciton coupling, as seen by a strong shift in the absorption spectrum, and hence exciton delocali-zation and migration. However, their structural integrity and hence their optical properties are very sensitive to their chemical environment as well as to mechanical deformation, rendering detailed studies on individual tubular J-aggregates difficult.

In a collaboration within the CRC 951 Hybrid Inorganic/Organic Systems for Opto-Electronics, projects A6 (Kirstein, Rabe) and A12 (Koch) we addressed this issue and developed a route for their chemical and mechanical stabilization by in situ synthesis of a silica coating that leaves their absorbance and emission unaltered in solution [1]. By electrostatic adsorption of precursor molecules, it was achieved to cover the aggregates with a silica shell of a few nanometer thickness which is able to stabilize the aggregates against changes of pH of solutions down to values where pure aggregates are oxidized, against drying under ambient conditions, and even against the vacuum conditions within an electron microscope. It was possible to measure spatially resolved electron energy loss spectra across a single freely suspended aggregate to analyze the chemical composition and the chemical composition and silica shell thickness.

The concept of electrostatic adsorption at the charged surface of the aggregates was also utilized for the adsorption of oppositely charged polyelectrolytes, polycations in this case [2]. It was found that the morphology of the resulting



Figure 1: Sketch of chemical structure of the amphiphilic carbocyanine C8S3 and the route to synthesize a closed shell of silica on top of the aggregates of the anionic carbocyanine by successive adsorption of the precursor molecules APTES and TEOS. The TEM images are taken at room temperature and show Room temperature silica coated aggregates deposited on a holey carbon film. The right image is a magnification showing a single aggregate, freely suspended across a hole.



Figure 2 Sketch of the tubular aggregates of C8S3 emphasizing the negative surface charge due to sulfonate end groups of the dye and chemical structure of the polycation PDADMAC. The Cryo-TEM image shows aggregates partially covered with PDADMAC.

aggregate/polycation complexes sensitively depends on the chemical structure of the polyelectrolyte. But in general, adsorption of a homogeneous layer leads to charge reversal of the surface of the complex, which can be used for further attachment of other chemicals. The adsorption of polyelectrolytes at these amphiphilic tubular structures, stabilized by means of hydrophobic forces, is far from obvious and demonstrates an applicable route to the hierarchical build-up of more complex nanostructures in solution by means of a self-assembling process.

- Individual tubular J-aggregates stabilized and stiffened by silica encapsulation
 K. Herman, H. Kirmse, A. Eljarrat, C.T. Koch,
 S. Kirstein, J.P. Rabe
 Colloid Polym Sci, 2020, 298(7), 937.
 doi: 10.1007/s00396-020-04661-0
- [2] Adsorption of polyelectrolytes onto the oppositely charged surface of tubular J aggregates of a cyanine dye

O. Al-Khatib, C. Böttcher, H. von Berlepsch, K. Herman, S. Schön, J.P. Rabe, S. Kirstein *Colloid Polym. Sci.*, 2019, 297(5), 729. doi: 10.1007/s00396-019-04487-5

Metal-Assisted and Solvent-Mediated Synthesis of Two-Dimensional Triazine Structures on Gram Scale

Covalent triazine frameworks are an emerging class of materials that have shown promising performance for a range of applications. In a large collaborative project, researchers from IRIS Adlershof together with their partners report on a metal-assisted and solvent-mediated reaction between calcium carbide and cyanuric chloride, as cheap and commercially available precursors, to synthesize two-dimensional triazine structures (2DTSs) [1]. The reaction between the solvent, dimethylformamide, and cyanuric chloride was promoted by calcium carbide and resulted in dimethylaminos-triazine intermediates, which in turn undergo nucleophilic substitutions. This reaction was directed into two dimensions by calcium ions derived from calcium carbide and induced the formation of 2DTSs. The role of calcium ions to direct the two-dimensionality of the final structure was simulated using DFT and further proven by synthesizing molecular intermediates. The water content of the reaction medium was found to be a crucial factor that affected the structure of the products dramatically. While 2DTSs were obtained under anhydrous conditions, a mixture of graphitic material/2DTSs or only graphitic material (GM) was obtained in aqueous solutions. Due to the straightforward and gram-scale synthesis of 2DTSs, as well as their photothermal and photodynamic properties, they are promising materials for a wide range of future applications, including bacteria and virus incapacitation.



Metal-assisted and solvent-mediated synthesis of twodimensional triazine structures on gram scale

A. Faghani, M.F. Gholami, M. Trunk, J. Müller, P. Pachfule, S. Vogl, I. Donskyi, P. Nickl, J. Shao, M.R.S. Huang, W.E.S. Unger, R. Arenal, C.T. Koch, B. Paulus, J.P. Rabe, A. Thomas, R. Haag, M. Adeli J. Am. Chem. Soc., 2020, 142(30), 12976. doi: 10.1021/jacs.0c02399

Reversible Switching of Charge Transfer at the Graphene-Mica Interface with Intercalating Molecules

Understanding and controlling charge transfer through molecular nanostructures at interfaces is of paramount importance, particularly for hybrid systems for optics and electronics but also generally for contact electrification or in bio-electronics. In a recent publication, Hu Lin et al. [1] reveal the influence of intercalation and exchange of molecularly thin layers of small molecules (water, ethanol, 2 propanol and acetone) on charge transfer at the well-defined interface between an insulator (muscovite mica) and a conductor (graphene) through probing graphene doping variations by Raman spectroscopy. While a molecular layer of water blocks charge transfer between mica and graphene, a layer of the organic molecules allows for it. The exchange of molecular water layers with ethanol layers switches the charge transfer very efficiently from OFF to ON and back. This observation is explained by charge transfer from occupied mica trap states to electronic states of graphene, controlled by the electrostatic potential from the molecular layers wetting the interface. This is

supported by molecular dynamics simulations. The sensitivity of graphene doping to the composition of confined molecular films may be used to investigate the structure of the films and diffusion of the molecules in the nano-confinement, *e.g.*, their miscibility; furthermore, potential molecular sensor and actuator applications can be



a) Schematic diagram of (i) an initially dry graphene-mica interface becoming intercalated with molecular (ii) ethanol or (iii) water layers, upon exposure to ethanol and water vapors, respectively. Water and ethanol molecules can diffuse into the interface and replace each other. b) Dependence of the graphene G peak position on time for alternating exposures to ethanol (green) and water vapor (blue). The light blue and red lines are G peak positions for unstrained/undoped and n-doped graphene on water and ethanol layers, respectively. 6. Scientific Highlights

envisioned. The demonstrated role of molecular layers in the charge transfer will aid in understanding of graphene wetting transparency, and it will facilitate the development of electronic devices, *e.g.*, triboelectric generators.

Reversible Switching of Charge Transfer at the Graphene-Mica Interface with Intercalating Molecules

H. Lin, J.-D. Cojal González, N. Severin, I.M. Sokolov, J.P. Rabe *ACS Nano*, 2020, 14(9), 11594. doi: 10.1021/acsnano.oco4144

HIDDEN SYMMETRIES IN MASSIVE QUANTUM FIELD THEORY

Theoretical models with a large amount of symmetry are ubiquitous in physics and often key to developing efficient methods for complex problems. If the number of symmetries surpasses a critical threshold, a system is called integrable with a prime example being the Kepler problem of planetary motion. While integrability typically comes with a rich spectrum of mathematical methods, it is often hard to identify the underlying symmetries. For the first time quantum integrability was now discovered in the context of massive quantum field theories in four spacetime dimensions. Florian Loebbert and Julian Miczajka (both IRIS Adlershof, HU Berlin) together with Dennis Müller (NBI Copenhagen) and Hagen Münkler (ETH Zürich) have shown that large classes of mostly unsolved massive Feynman integrals feature an infinite dimensional Yangian symmetry - a hallmark of integrability. This mathematical structure is highly

constraining and it allows to completely fix these building blocks of quantum field theory as has been demonstrated for first examples. The observed Yangian symmetry goes hand in hand with an extension of the important structure of conformal



Massive Conformal Symmetry and Integrability for Feynman Integrals

F. Loebbert, J. Miczajka, D. Müller, and H. Münkler Phys.Rev. Lett. 125 (2020) 9, 091602. doi: 10.1103/PhysRevLett.125.09160

UNDERSTANDING THE INTERACTION OF POLYELECTROLYTE ARCHITECTURES WITH PROTEINS AND BIOSYSTEMS



Interaction of polyelectrolytes with biosystems at different levels of complexity. The entire matrix of systems and problems surveys the possible medical problems to which synthetic polyelectrolytes may provide solutions

Polyelectrolytes such as e.g. DNA or heparin are long linear or branched macromolecules onto which charges are appended. The counterions neutralizing these charges mav dissociate in water and will largely determine the interaction of such polyelectrolytes with biomolecules and in particular with proteins. Here Prof. Matthias Ballauff. member of IRIS Adlershof, and colleagues review studies on the interaction of proteins with polyelectrolytes and how this knowledge can be used for medical applications. Counterion release was identified as the main driving force for the binding of proteins to polyelectrolytes: Patches of positive charge become multivalent counterions of the polyelectrolyte

which leads to the release of counterions of the polyelectrolyte and a concomitant increase of entropy.

This was shown by surveying investigations done on the interaction of proteins with natural and synthetic polyelectrolytes. Special emphasis is laid on sulfated dendritic polyglycerols (dPGS). The entire overview demonstrates that we are moving on to a better understanding of charge-charge interaction in system of biological relevance. Hence, research along these lines will aid and promote the design of synthetic polyelectrolytes for medical applications.

Understanding the interaction of polyelectrolyte architectures with proteins and biosystems

K. Achazi, R. Haag, M. Ballauff, J. Dernedde, J.N. Kizhakkedathu, D. Maysinger, and G. Multhaup *Angew. Chem. Intl Ed*, 2020, 60(8), 3882. doi:10.1002/anie.202006457



Interaction of proteins with highly charged polyelectrolytes as *e.g.* DNA by counterion release

Printed perovskite LEDs – an innovative technique towards a new standard process of electronics manufacturing

A team of researchers from the Helmholtz-Zentrum Berlin (HZB) and Humboldt-Universität zu Berlin has succeeded for the first time in producing light-emitting diodes (LEDs) from a hybrid perovskite semiconductor material using inkjet printing. This opens the door to broad application of these materials in manufacturing many different kinds of electronic components. The scientists achieved the breakthrough with the help of a trick:

"inoculating" (or seeding) the surface with specific crystals.

Microelectronics utilize various functional materials whose properties make them suitable for specific applications. For example, transistors and data storage devices are made of silicon, and most photovoltaic cells used for generating electricity from sunlight are also currently made of this semiconductor material. In contrast, compound semiconductors such as gallium nitride are used to generate light in optoelectronic elements such as light-emitting diodes (LEDs). The manufacturing processes also different for the various classes of materials.

Transcending the materials and methods maze

Hybrid perovskite materials promise simplification – by arranging the organic and inorganic components of semiconducting crystal in a specific structure. "They can be used to manufacture all kinds of microelectronic components by modifying their composition", says Prof. Emil List-Kratochvil, head of a Joint Research Group at HZB and Humboldt-Universität zu Berlin. What's more, processing perovskite crystals is comparatively simple. "They can be produced from a liquid solution, so you can build the desired component one layer at a time directly on the substrate", the physicist explains.

First solar cells from an inkjet printer, now light-emitting diodes too

Scientists at HZB have already shown in recent years that solar cells can be printed from a solution of semiconductor compounds – and are worldwide leaders in this technology today. Now for the first time, the joint team of HZB and HU Berlin has succeeded in producing functional light-emitting



A look inside the Helmholtz Innovation Lab HySPRINT. Major work on the printable perovskite-LEDs was carried out here. \bigcirc HZB/Phil Dera

diodes in this manner. The research group used a metal halide perovskite for this purpose. This is a material that promises particularly high efficiency in generating light – but on the other hand is difficult to process. "Until now, it has not been possible to produce these kinds of semiconductor layers with sufficient quality from a liquid solution", says List-Kratochvil. For example, LEDs could be printed just from organic semiconductors, but these provide only modest luminosity. "The challenge was how to cause the salt-like precursor that we printed onto the substrate to crystallise quickly and evenly by using some sort of an attractant or catalyst", explains the scientist. The team chose a seed crystal for this purpose: a salt crystal that attaches itself to the substrate and triggers formation of a gridwork for the subsequent perovskite layers.

Significantly better optical and electronic characteristics

In this way, the researchers created printed LEDs that possess far higher luminosity and considerably better electrical properties than could be previously achieved using additive manufacturing processes. But for List-Kratochvil, this success is only an intermediate step on the road to future microand optoelectronics that he believes will be based exclusively on hybrid perovskite semiconductors. "The advantages offered by a single universally applicable class of materials and a single cost-effective and simple process for manufacturing any kind of component are striking", says the scientist. He is therefore planning to eventually manufacture all important electronic components this way in the laboratories of HZB and HU Berlin. List-Kratochvil is Professor of Hybrid Devices



Graphical representation of the printing process for the perowskite-LEDs. © C. Rothkirch/HU Berlin

at the Humboldt-Universität zu Berlin and head of a Joint Lab founded in 2018 that is operated by HU together with HZB. In addition, a team jointly headed by List-Kratochvil and HZB scientist Dr. Eva Unger is working in the Helmholtz Innovation Lab HySPRINT on the development of coating and printing processes – also known in technical jargon as "additive manufacturing" – for hybrid perovskites. These are crystals possessing a perovskite structure that contain both inorganic and organic components.

Finally, inkjet-printed metal halide perovskite LEDs – utilizing seed crystal templating of salty PEDOT:PSS

F. Hermerschmidt, F. Mathies, V.R.F. Schröder,

C. Rehermann, N. Zorn Morales, E.L. Unger, E.J.W. List-Kratochvil.

Mater. Horiz., 2020(7), 1773. doi: 10.1039/DoMH00512F

MODULATING THE LUMINANCE OF ORGANIC LIGHT-EMITTING DIODES VIA OPTICAL STIMULATION OF A PHOTOCHROMIC MOLECULAR MONOLAYER AT TRANSPARENT OXIDE ELECTRODE

Organic self-assembled monolayers (SAMs) deposited on inorganic bottom electrodes are commonly used to tune charge carrier injection or blocking in hybrid inorganic/organic optoelectronic devices. Beside the enhancement of device performance, the fabrication of multifunctional devices in which the output can be modulated by multiple external stimuli remains a challenging target. The authors of



a) Luminance of an OLED fabricated with a SAM-modified ITO electrode. The luminescence doubles once the DAE is switched from closed to open.

b) Values for the ratio between the current densities and luminescence measured at 5 V upon multiple irradiation cycles. The modulation of the OLED luminescence is reversible. this research highlight report the functionalization of an indium tin oxide (ITO) electrode with a SAM of a photochromic diarylethene derivative designed for optically control the electronic properties. Following the demonstration of dense SAM formation and its photochromic activity, as a proof-ofprinciple, an organic light-emitting diode (OLED) embedding the light-responsive SAM-covered electrode is fabricated and characterized. Optically addressing the twoterminal device by irradiation with ultraviolet light (315 nm) doubles the electroluminescence (100% gain), which can be reversed by irradiation with visible light (530 nm). This approach of "dynamic" energy tuning could be successfully exploited in the field of opto-communication technology, for example to fabricate opto-electronic logic circuits.

Modulating the luminance of organic light-emitting diodes via optical stimulation of a photochromic molecular monolayer at transparent oxide electrod

G. Ligorio, G. F. Cotella, A. Bonasera, N. Zorn Morales, G. Carnicella, B. Kobin, Q. Wang, N. Koch, S. Hecht, E.J.W. List-Kratochvil, and F. Cacialli *Nanoscale* 2020, 12(9), 5444. doi: 10.1039/donro0724b

Review on hybrid integrated quantum photonic circuits

Recent developments in chip-based photonic quantum circuits have radically impacted quantum information processing. However, it is challenging for monolithic photonic platforms to meet the stringent demands of most quantum applications. Hybrid platforms combining different photonic technologies and different materials in a single functional unit have great potential to overcome the limitations of monolithic photonic circuits.

Researchers from the KTH Royal Institute of Technology, Stockholm, Sweden, the University of Muenster, Germany, the National Institute of Standards and Technology, Gaithersburg, USA, and IRIS Adlershof review the progress of hybrid quantum photonics integration. They discuss important design considerations, including optical connectivity and operation conditions, and outline the roadmap for realizing future advanced large-scale hybrid devices, beyond the solid-state platform, which hold great potential for quantum information applications.



Three examples of hybrid integration: (a) Dibenzoterrylene embedded in a rigid matrix of crystalline anthracene as molecule singlephoton source on a silicon nitride waveguide [Lombardi, et al. ACS Photon. 5, 126–132 (2018)], (b) Nonlinear phase gate in a hybrid atomic-photonic system [Tiecke, et al., Nature 508, 241–244 (2014)], (c) Hybrid atomic cladding photonic waveguide demonstrating light-matter interaction at room temperature [Stern, et al., Nat. Commun. 4, 1548 (2013)].

Hybrid integrated quantum photonic circuits

A.W. Elshaari, W. Pernice, K. Srinivasan, O. Benson and V. Zwiller Nat. Photonics, 2020, 14(5), 285. doi: 10.1038/s41566-020-0609-x

Excited-state charge transfer enabling $MoS_2/Phthalocyanine$ photodetectors with extended spectral sensitivity

The combination of inorganic monolayer (ML) transitionmetal dichalcogenides (TMDCs) with organic semiconductors holds the promise to further improve opto-electronic device properties with added functionality. The authors of this research highlight investigate a hybrid inorganic/organic system (HIOS) consisting of metal-free phthalocyanine (H₂Pc) as thin organic absorber layer and ML MoS₂ as TMDC. Via a combination of photoemission (PES), photoluminescence (PL), and photocurrent action spectroscopy they demonstrate, that excited-state charge transfer from the H2Pc layer enhances the photo response of ML MoS₂ without loss in sensitivity extended to spectral regions where the TMDC is transparent. This observation is explained by the staggered type II energy-level alignment at the hybrid interface facilitating efficient exciton dissociation and excitedstate charge transfer with the holes residing in the H₂Pc HOMO and the electrons in the MoS₂ conduction band. In hybrid photodetectors, these transferred charges increase the concentration of carriers in MoS₂ and with that its photoconductivity. The present demonstration of a highly





efficient carrier generation in TMDC/organic hybrid structures paves the way for future nanoscale photodetectors with very wide spectral sensitivity.

(a) Schematic design of the hybrid H_2Pc/MOS_2 photodetecting device. H_2Pc layer thickness is $dH_2Pc = 3.0$ nm (b) Photoresponse of the hybrid (blue) and the reference MoS2-only (red) device. The spectra were normalized at the spectral position where H_2Pc does not absorb, *i.e.*, ~ 2.5 – 2.55 eV. The difference (green) between the spectra of the hybrid and reference devices.

Excited-State Charge Transfer Enabling MoS₂/Phthalocyanine Photodetectors with Extended Spectral Sensitivity

N. Mutz, S. Park, T. Schultz, S. Sadofev, S. Dalgleish, L. Reissig, N. Koch, E.J.W. List-Kratochvil, S. Blumstengel J. Phys. Chem. C, 2020, 124(5), 2837. doi: 10.1021/acs.jpcc.9b10877

INSIGHTS INTO CHARGE TRANSFER AT THE ATOMICALLY PRECISE NANOCLUSTER/SEMICONDUCTOR INTERFACE FOR IN-DEPTH UNDERSTANDING THE ROLE OF NANOCLUSTER IN PHOTOCATALYTIC SYSTEM



(a) Schematic illustration of the H2 production by Ag_{44} -TiO₂ under simulated sunlight; (b) Catalytic performance of TiO₂ (black), Ag NP-TiO₂ (yellow) and Ag_{44} -TiO₂ (red).

A TiO₂/cluster composite of type II junction configuration for photocatalytic hydrogen evolution is built by deposition of atomically precise Ag₄₄ nanocluster on TiO₂. Besides photosensitizer, the cluster is found to serve as co-catalyst to improve the charge separation efficiency of the system, which is quite different from the well-known plasmonic nanoparticle enhanced systems. The hydrogen production rate by Ag_{44} -TiO₂ is ten times higher than that of the pure TiO₂ and five times higher than that of the Ag NP-TiO₂.

Insights into charge transfer at the atomically precise nanocluster/semiconductor interface for in-depth understanding the role of nanocluster in photocatalytic system

Y. Wang, X-H. Liu, Q. Wang, M. Quick, A.S. Kovalenko, Q.-Y. Chen, N. Koch, and N. Pinna *Angew. Chem. Int. Ed.*, 2020, 59(20), 7748. doi: 10.1002/anie.201915074

INFLUENCE OF INTERFACE HYDRATION ON SLIDING OF GRAPHENE AND MOLYBDENUM-DISULPHIDE SINGLE-LAYERS



Strain transfer measurements for both a) dry and b) hydrated graphene-mica interfaces: the surface of the mica substrate was strained by bending the mica slab in steps. Strains in graphene were followed with Raman peak positions. Strain relaxation in graphene changes from stick-slip in dry contact, to viscous when hydrated.

Humidity influences friction in layered materials in peculiar ways. For example, while water improves the lubricating properties of graphite, it deteriorates those of molybdenum disulphide (MoS₂). The reasons remain debated, not the least due to the difficulty to experimentally compare dry and hydrated interface frictions. Hu Lin et al. [1] have shown that the hydration of interfaces between a mica substrate and single-layers of graphene and MoS₂ with a molecularly thin water layer affects strain transfer from the substrate to the 2D materials. For this, the substrate has been strained and the strain in graphene and MoS₂ has been detected by changes in Raman and photoluminescence spectra, respectively. Graphenes on dry mica exhibit "stick-and-slip" strain relaxation with frictional forces per area of up to about 100 kPa. Strains relaxation in hydrated graphenes is viscous with estimated viscous friction coefficients in units of force per unit area and per unit velocity of about 1.10¹⁷ Pa.s/m. In contrast, there is no viscous relaxation in MoS2 regardless of hydration. This work provides a novel approach for better understanding the impact of hydration on friction in layered materials

Influence of interface hydration on sliding of graphene and molybdenum-disulfide single-layers

H. Lin, A. Rauf, N. Severin, I.M. Sokolov, J.P. Rabe J. Colloid Interface Sci., 2019, 540, 142. doi: 10.1016/j.jcis.2018.12.089

OFF-SHELL GAUGE INVARIANCE



Master integrals for reduction of 4-point functions

Dirk Kreimer (IRIS member), John Gracey (U. Liverpool and DFG Mercator Fellow in Kreimer's group) and postdoc Henry Kissler could clarify the algebraic and combinatorical foundations of off-shell Slavnov Taylor identities, off-shell gauge invariance that is. The problem remained open in the litera- ture for many years and was now settled by modern algebra and confirmed computation- ally. Quantum chromodynamics served here as a concrete test case. Generalizations to other gauge theories are under study.

Using Hopf-algebraic structures as well and diagrammatic techniques for determining the Slavnov-Taylor identities for QCD familiar from the study of graph complexes we construct relations for off-shell Green functions. The methods are sufficiently versatile to allow for applications even in the study of diffeomorphism invariance in quantum gravity in the future.

Self-consistency of off-shell Slavnov-Taylor identities in QCD

J. A. Gracey, H. Kißler, and D. Kreimer *Phy. Rev. D*, 2019, 100(8-15), 85001. doi: 10.1103/PhysRevD.100.085001

"SPACE – TIME – MATTER: Analytic and Geometric Structures": A Book about CRC 647 results published

This monograph describes some of the most interesting results obtained by the mathematicians and physicists collaborating in the CRC 647 "Space – Time – Matter", in the years 2005 - 2016. It concerns the mathematical and physical foundations of string and quantum field theory as well as cosmology. The work starts with an excellent introduction by the editors Jochen Brüning and Matthias Staudacher, both



members of IRIS Adlershof, that gives an historical overview of the field and vividly retells the development of the CRC. Then each project of the final funding period is summarized and also represented in detail by the following 15 chapters, many contributed by IRIS scientists:

- o Dyson-Schwinger equations: Fix-point equations for quantum fields by Dirk Kreimer (IRIS member)
- Hidden structure in the form factors of N = 4 SYM by Dhritiman Nandan (former member at AG Staudacher) and Gang Yang
- On regulating the AdS superstring by Valentina Forini (IRIS Junior member)
- Yangian symmetry inmaximally supersymmetric Yang-Mills theory by Livia Ferro, Jan Plefka (IRIS member), and Matthias Staudacher (IRIS member)
- Geometric analysis on singular spaces by Francesco Bei (former member at AG Brüning), Jochen Brüning (IRIS member), Batu Güneysu (former IRIS young researcher and member at AG Brüning), and Matthias Ludewig

SPACE – TIME – MATTER: Analytic and Geometric Structures

Jochen Brüning, Matthias Staudacher (Eds.) DOI: 10.1515/9783110452150 ISBN (print): 978-3-11-045135-1 ISBN (PDF): 978-3-11-045215-0 ISBN (epub): 978-3-11-045153-5

Entangled Photons for Mid-Infrared Sensing – Quantum Futur Award 2019 for Aron Vanselow

Aron Vanselow receives the second prize of the Quantum Futur Award 2019, sponsored by Ministry of Science and Education for his master thesis at Humboldt-Universität zu Berlin.

It has long been anticipated that entangled photons hold the promise to drive a paradigm shift in imaging and sensing. Realworld implementations, however, have lagged behind their classical counterparts, because of low efficiency, loss and decoherence.

Vanselow's thesis, carried out in the junior research group "Nonlinear Quantum Optics", led by Dr. Sven Ramelow, who is a member of IRIS Adlershof, presents the first experimental demonstration of mid-infrared frequency-domain optical coherence tomography (OCT) with entangled photons. OCT is an



Working principle underlying (ai) classical FD-OCT and (aii) FD-OCT with undetected photons.

important depth-imaging method in biomedical diagnostics as well as non-destructive testing allowing for 3D microscopy. OCT in the mid-IR range enables looking inside strongly scattering media, where commercial systems which are all at shorter wavelengths don't work.

The proof-of-principle setup developed by Vanselow, Ramelow and their colleagues is powered by quantum entanglement generated in a patented new crystal. Importantly, the reached performances are already comparable to the best conventional techniques while exposing the sample to 8 orders of magnitude less optical power. At the same time the technological overhead is drastically reduced compared with classical techniques using only compact and cost-effective components.

With this thesis demonstrating fast 2D and 3D imaging of highly scattering real-world samples (ceramics, paint layers) with 20 μ m lateral and 10 μ m depth resolution it has immediate relevance for applications in non-destructive testing such as quality control of coating thicknesses, cultural heritage conservation and microfluidics.

Mid-infrared Frequency-domain Optical Coherence Tomography with Undetected Photons

A. Vanselow, P. Kaufmann, I. Zorin, B. Heise, H. Chrzanowski, and S. Ramelow In: Proceedings Quantum Information and Measurement (QIM) V: Quantum Technologies. Optical Society of America. ISBN-978-1-943580-56-9, 2019

Ultra-broadband SPDC for spectrally far separated photon pairs

A. Vanselow, P. Kaufmann, H. M. Chrzanowski, and S. Ramelow *Optics Letters*, 2019, 44(19), 4638. doi: 10.1364/OL.44.004638

DIRECT MEASUREMENT OF QUANTUM EFFICIENCY OF SINGLE-PHOTON EMITTERS IN HEXAGONAL BORON NITRIDE

Two-dimensional materials like boron nitride (h-BN) have recently attracted the attention of the quantum optics and nano optics community. Individual single photon emitting (SPE) defects can be found even in single layers of h-BN. These emitters are bright and stable and have a narrow emission line, making them potentially suitable for use in quantum communication devices. As the field is still young, it is difficult to create SPEs with desired properties. One reason for this is the yet unknown atomic origin of the defect, which could help to identify processing steps that could lead to the desired outcome. In order to determine the atomic origin of an emitter, calculations are carried out under the



assumption of different atomic configurations and compared with the observed spectra. Unfortunately, the h-BN SPEs spectra are distributed over a wide range, which makes the application of this method difficult. Another intrinsic property is the quantum efficiency (QE), *i.e.* the branching ratio between a radiative rate and the total (radiative and non-radiative) decay rate.

Researchers of Nanooptik AG of Humboldt-Universität zu Berlin in cooperation with the Technical University of Sydney could now directly measure the absolute QE of single defects in h-BN. The underlying principle is based on the proportionality between a controlled change in the local density of the states into which the emitter can emit and the lifetime of the excited state. The researchers implemented this experimentally by controlling the distance between the SPE and a mirror with nanometer accuracy while measuring the lifetime of the excited state. In this way, not only the high QE of up to $87 \pm$ 7% was determined, but also a correlation between fluorescence wavelength and QE was found. This paves the way for a better understanding of the origin of the emitters.



Schematics of the performed experiment and a distance dependent lifetime measurement. (a) The AFM is equipped with a goldcoated hemispherical tip aligned with an SPE in h-BN and held at a variable distance. The objective lens on the bottom of the glass excites the SPE (green pulsed laser) and collects its emission. With this setup, distance-dependent lifetime measurements can be performed, one such measurement is shown in (b) (points). To determine the QE, an adjustment was performed (blue solid line). The same fit function with a QE of 1.0 is represented by the green solid line as a reference.

Direct measurement of quantum efficiency of single-photon emitters in hexagonal boron nitride

N. Nikolay, N. Mendelson, E. Özelci, B. Sontheimer, F. Böhm, G. Kewes, M. Toth, I. Aharonovich, and O. Benson Optica, 2019, 6(8), 1084. doi: 10.1364/OPTICA.6.001084
Article of IRIS junior research group leader Michael J. Bojdys published in Nature Communications

The IRIS junior research group leader Michael J. Bojdys and his international team have achieved a great success: Their article "Real-time optical and electronic sensing with a β amino enone linked, triazine-containing 2D covalent organic framework" has been selected to be published in the renowned journal Nature Communications.



Bojdys article deals with aromatic two-dimensional covalent organic frameworks (2D COFs), which are a class of porous polymers that allow the precise incorporation of organic units into periodic structures. COFs can be chemically designed to incorporate particular surface functional groups which can be exploited to tune the optical and electronic properties. However, low stability towards chemical triggers has hampered their practical implementations.

Together with a team from the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (Prague, Czech Republic), IRIS junior research group leader Michael I. Boidvs and his team from Humboldt-Universität zu Berlin have explored a new design principle for COFs that makes use of strong, overall conjugation and incorporation of donor-acceptor domains. In this study a new, a highly stable chemoresistant β-amino enone linked, triazine-containing COF was used as a real-time, reversible optical and electronic sensor for volatile acids and bases. The team was further able to conclude that the sensing capabilities of the COF was achieved by preferential protonation of the electron accepotor – a triazine ring in the structure –, resulting in an optical response visible to the naked eye and an increase of bulk electrical conductivity by two orders of magnitude. These findings demonstrate a powerful approach to design

more practical sensors and switches, and take genuine advantage of the chemoresistant make-up, porous structure, and overall conjugation of fully-aromatic systems. Real-time optical and electronic sensing with a β -amino enone linked, triazine-containing 2D covalent organic framework

R. Kulkarni, Y. Noda, D.K Barange, Y.S. Kochergin, P. Lyu, B. Balcarova, P. Nachtigall, and M.J. Bojdys *Nat. Commun*, 2019, 10(1), 3228. doi: 10.1038/s41467-019-11264-z

A NOVEL SEMICONDUCTOR FROM THE FAMILY OF CARBON NITRIDES

Research teams from the Humboldt-Universität and the Helmholtz Zentrum Berlin (HZB) have investigated a new material from the family of carbon nitrides. Triazine-based graphitic carbon nitride (TGCN) is a semiconductor that is useful in optoelectronic applications. Its structure is two-dimensional and layered, and it resembles that of graphene. Unlike graphene, its conductivity between the layers is 65times higher than in-plane.

Some organic materials can be used in optoelectronics just like silicon-based semiconductors. Whether in solar cells, light-emitting diodes, or as transistors – the important property is the bandgap, *i.e.* the energy-difference of the electrons in the valence band and the conduction band. The basic principle underlying all electronic components is that electrons



can be promoted by light or by voltage between the valence and the conduction band. Here, bandgaps between 1 and 2 eV are ideal.

A team led by the chemist Dr. Michael J. Bojdys from the chemistry department and IRIS Adlershof of the Humboldt-Universität zu Berlin, has recently synthesized an organic semiconductor from the family of carbon nitrides. This triazine-based graphitic carbon nitride (TGCN) consists exclusively from carbon and nitrogen atoms and can be grown as a brown film on quartz glass substrates. The C- and N-atoms connect in hexagonal, honeycomb patterns like carbon atoms in graphene. Just like in graphene, the crystal structure of TGCN is based on layered, two-dimensional sheets. In graphene, in-plane conductivity is excellent, however, it is much lower through the planes. In the case of TGCN, the opposite is observed: through-plane conductivity is 65-times higher than in-plane. With a bandgap of 1.7 eV TGCN is a good candidate for optoelectronic applications.

The HZB-physicist Dr. Christoph Merschjann has examined the charge carrier transport in samples of TGCN using timeresolved absorption measurements in the femto- to nanosecond regime at the laser lab JULiq – a joint lab between the HZB and the Freie Universität Berlin. Such laser experiments offer a unique way to correlate macroscopic conductivity and microscopic transport models. From his measurements, he was able to deduce how the charge carriers diffuse throughout the material. "Electrons do not exit the hexagonal honeycombs of triazine units horizontally, but they move at a slope to the nearest triazine-unit in the neighboring layer. The crystal structure of the material leads to a preferred movement of charge carriers along tube-like channels." This mechanism could explain why the conductivity of TGCN is fundamentally higher through-plane than in-plane. "TGCN is the hitherto best candidate to replace silicon semiconductors and the critical, rare-earth dopants used in their manufacture", says Michael Bojdys. "The production method for TGCN that we developed in my group at the Humboldt-Universität zu Berlin yields flat layers of semiconducting TGCN on insulating quartz glass. This enables relatively easy upscaling and device production."

Directional charge transport in layered, two-dimensional triazine-based graphitic carbon nitride

Y. Noda, C. Merschjann, J. Tarábek, P. Amsalem, N. Koch, and M.J. Bojdys *Angew. Chem. Int. Ed.*, 2019, 58(28), 9394. doi: 10.1002/anie.201902314

Researchers demonstrate very large electric tuning of a single quantum emitter at room temperature

Bright and tunable solid-state single-photon emitters (SPEs) are required for the realization of scalable quantum photonic technologies. Recently, optically active defects in a two-dimensional material, boron nitride (h-BN), have been extensively studied as bright single-photon emitters with a narrow linewidth and operating at room temperature. The layered nature of h-BN also offers potential advantages for integration in novel opto-electronic hybrid elements including photonic resonators, waveguides, modulator, and detectors. In order to exploit the functionality of such elements a tuning of the emitter's fluorescence line is essential. Tuning via the Stark effect using a static electric field has been suggested for various solid-state emitters, such as quantum dots or color centers in diamond. Researcher from the Institute of Physics of Humboldt-University together with coworkers from the University of Technology in Sydney were now able to demonstrate controlled and reversible Stark tuning of individual emitters in hBN. They used a metallic tip of an atomic force microscope (AFM) to locally select a single emitter and tune it over a record range of up to 5.5 nanometers at room temperature.



a) Structure of a defect in hexagonal Boron Nitride. b) Schematic of the experiment, where a metallic AFM tip is placed above a single defect emitter and a bias voltage is applied.c) Measured Stark-shift of the narrow fluorescence line.

Based on their results the researchers suggest building a room-temperature single photon source, which can be tuned electrically in or out of a resonance of a plasmonic resonator. "Such a source would be highly desirable as a reliable nonclassical light source for applications in quantum-enhanced sensing and metrology or in quantum key distribution." says Prof. Oliver Benson, who is researcher in IRIS Adlershof and leads the Humboldt-team.

Very large and Reversible Stark-Shift Tuning of Single Emitters in Layered Hexagonal Boron Nitride

N. Nikolay, N. Mendelson, N. Sadzak, F. Böhm, T.T. Tran, B. Sontheimer, I. Aharonovich, O. Benson Phys. Rev. Applied, 2019, 11(4), 41001. doi: 10.1103/PhysRevApplied.11.041001

ENLIGHTENING FULL-COLOR DISPLAYS

Researchers from the University of Strasbourg & CNRS (France), in collaboration with University College London (United Kingdom), and Humboldt-Universität zu Berlin (Germany), have shown that a subtle combination of lightemitting semiconducting polymers and small photoswitchable molecules can be used to fabricate light-emitting organic transistors operating under optical remote control, paving the way to the next generation of multifunctional optoelectronic devices. These achievements have now been published in Nature Nanotechnology. Organic light-emitting transistors are widely recognized as key components in numerous optoelectronic applications. However, the integration of multiple functionalities into a single electronic device remains a grand challenge in this technological sector. Moreover, the next generation of displays requires to encode high-density visual information into single and ultra-



small pixels. Now a team of researchers from Strasbourg, London, and Berlin has taken a big step forward by creating the first organic light-emitting transistor that can be remotecontrolled by light itself. They have been blending a customdesigned molecule as a miniaturized optical switch with a light-emitting semiconducting polymer. Upon illumination with ultraviolet and visible light, the molecular switch reversibly changes its electronic properties. As a consequence, the electrical and optical response of the device can be modulated simultaneously by light, which serves as an optical remote control. However, having a device capable of producing only one color is not sufficient for daily-life applications, such as full-color displays. By choosing appropriate photoswitchable molecules and blending them with suitable light-emitting polymers, the researchers have demonstrated that this new type of organic light-emitting transistors can shine in the range of the three primary colors (red, green, and blue), thereby covering the entire visible spectrum. The disruptive potential of such approach was demonstrated by writing and erasing spatially defined emitting patterns (a letter for example) within a single device with a beam of laser light, allowing a non-invasive and mask-free process, with a response time on the microsecond scale and a spatial resolution of a few micrometers, thus outperforming the best "retina" displays. Clearly, these findings represent a major breakthrough that offers multiple perspectives for smart displays, active optical memories, and light-controlled logic circuits.

Optically switchable organic light-emitting transistors

L. Hou, X. Zhang, G.F. Cotella, G. Carnicella, M. Herder, B.M. Schmidt, M. Pätzel, S. Hecht, F. Cacialli, and P. Samorì *Nature Nanotechnology*, 2019, 14(4), 347. doi: 10.1038/s41565-019-0370-9

Hybrid Organic-Inorganic Perovskites: Promising Substrates for Single-Atom Catalysts

Mononuclear metal species are widespread in enzymes and homogeneous catalysts. When such isolated single metal atoms are placed on a solid surface, they can also play an important role in heterogeneous catalysis. In the past few years, great attention has been paid to single-atom catalysts, not only because they can exhibit superior catalytic performance, but also, because they offer a novel way of maximizing the efficiency of utilizing atoms, which is especially desirable in the use of scarce metal elements like platinum. However, single atoms cannot work in isolation but need to be dispersed on suitable substrates.



Qiang Fu and Claudia Draxl have recently demonstrated that hybrid organic-inorganic perovskites - the emerging candidates in solar-cell applications - are highly promising substrates for Pt single atom catalysts. Through systematic first-principles calculations, they found that single Pt atoms are stabilized on such substrates through a synergistic cooperation between covalent bond formation and charge transfer. The generated Pt sites possess excellent catalytic properties in CO oxidation and may be able to play a role in CO2 reduction. This work not only has promising consequences in single -atom catalysis but also sheds light on potential applications of hybrid perovskites as photocatalysts.

Hybrid Organic-Inorganic Perovskites as Promising Substrates for Pt Single-Atom Catalysts

Q. Fu and C. Draxl *Physical Review Letters*, 2019, 122(4), 46101. doi: 10.1103/PhysRevLett.122.046101

AB INITIO MODELING OF NOVEL PHOTOCATHODE MATERIALS FOR HIGH BRIGHTNESS ELECTRON BEAMS



The development of laser-driven photocathode radio-frequency electron injectors has become a significant enabling technology for free electron lasers and for the fourth generation of light sources. Such remarkable progress come with quest for novel materials that are able to operate in the visible region with optimized quantum efficiency and minimized intrinsic emittance. Multi-alkali antimonides have recently emerged as ideal materials for photocathode applications in spite of the little fundamental knowledge regarding their electronic and optical properties. A team composed of scientists from the HU Berlin and HZB carried out a systematic investigation of the electronic structure and excitations of C_sK_2Sb , an exemplary and promising multi-alkali antimonide, by means of first-principles many-body methods. The results of their study confirm that this material is an excellent candidate for photocathode applications and pioneers a new research line bridging solid-state theory, material science, and accelerator physics in view of an improved modelling and design of materials for the next-generation electron sources.

This work was published on *The Journal of Physics: Condensed Matter* as an invited contribution to Prof. Caterina Cocchi, a member of IRIS Adlershof since 2017, to the special issue "Emerging leaders 2018".

First-principles many-body study of the electronic and optical properties of CsK2Sb, a semiconducting material for ultra-bright electron sources

C. Cocchi, S. Mistry, M. Schmeißer, J. Kühn, and T. Kamps J. Phys. Condens. Matter, 2019, 31(1), 14002. doi: 10.1088/1361-648X/aaedee

7. APPENDIX

7.1. IRIS-PUBLICATIONS IN HIGH IMPACT JOURNALS

Science Family

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I. Kviatkovsky, H.M. Chrzanowski, E.G. Avery, H. Bartolomaeus, and S. Ramelow, "Microscopy with undetected photons in the mid-infrared", *Science Advances*, 2020, 6(42), eabdo264. doi: 10.1126/sciadv.abdo264

NATURE FAMILY

R. Kulkarni, Y. Noda, D. Kumar Barange, Y.S. Kochergin, P. Lyu, B. Balcarova, P. Nachtigall, and M.J. Bojdys, "Realtime optical and electronic sensing with a β -amino enone linked, triazine-containing 2D covalent organic framework", *Nature Communications*, 2019, 10(1). doi: 10.1038/s41467-019-11264-z M. Regehly, Y. Garmshausen, M. Reuter, N.F. König, E. Israel, D.P. Kelly, C.-Y. Chou, K. Koch, B. Asfari, and S. Hecht, "Xolography for linear volumetric 3D printing", *Nature*, 2020, 588(7839), 620. doi: 10.1038/s41586-020-3029-7

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A. Wadle, V.W.-W. Yam, and Y.-W. Yang, "A Diverse View of
Science to Catalyse Change", *Journal of the American Chemical Society*, 2020, 142(34), 14393. doi: 10.1021/jacs.oco7877

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7.2. PATENTS

Title	Patent number	Status	Year	Involved member
Anode und Verfahren zu ihrer Herstellung	DE 10 2019 110 450 & IPC H01M 4/137	granted	2020	Bojdys
Verfahren und Einrichtung zur Frequenzumsetzung	DE 10 2017 223 197 B3	granted	2019	Benson
Verfahren zum Herstellen eines Bauelements, Bauelement und Verwendung des Bauelements, based on "Ultra-broadband SPDC for spectrally far separated photon pairs"	DE 10 2018 206 810.0	granted	2019	Ramelow
Struktursystem zum Aufbau photonischer in- tegrierter Schaltkreise und Verfahren zu dessen Herstellung	DE 10 2018 108 114.6	granted	2019	Ramelow

7.3. IRIS RELATED SPIN-OFFS

Name of founder	Name of spin-off company	Financed by	Year
Stefan Hecht	xolo GmbH	venture capital	2019

7.4. Awards, Academic Prizes, and Honors

Award	Awardee
Chairman of the Physikalische Gesellschaft zu Berlin (2020)	Oliver Benson
ERC 'Proof of Concept' Grant (2020)	Michael J. Bojdys (Bojdys)
Election as member of Academia Europaea (2020)	Stefan Hecht
Fischer-Nernst-Studienpreis des Instituts für Chemie der HU (2020)	Max Heyl (List-Kratochvil)
Albert-Weller-Preis der Fachgruppe Photochemie der Gesellschaft Deutscher Chemiker und der Bunsengesellschaft (2020)	Michael Kathan (Hecht)
Friedrich Hirzebruch Dissertation Prize of the Studienstiftung des deutschen Volkes (2020)	Michael Kathan (Hecht)
Postdoctoral fellowship of the Alexander von Humboldt-Foundation (2020)	Jie Li (Hecht)
Scientific Advisory Board Member of the Max Planck Institute for Chemical Energy Conversion (MPI-CEC) (2020)	Christian Limberg
Humboldt Research Fellowship for Postdoctoral Researchers (2020)	Joseph Munns (Schröder)
DGaO-Nachwuchspreis 2020	Aron Vanselow (Ramelow)
Distinguished guest professor at UTS Sydney, Australia (2019)	Oliver Benson

Appointment as Fellow of the Max Planck Society within the Graduate Cen- ter for Quantum Materials (2019)	Claudia Draxl
Chercheur invité international at Ecole Normale Supérieure, Paris (2019)	Thomas Elsässer
ERC Advanced GrantERC Advanced Grant BIOVIB (2019)	Thomas Elsässer
Einstein Junior Fellowship (2019)	Valentina Forini
Symposium IRIS 2019: Best-Poster-Award	Benedikt Haas (KochC)
Communication Award sponsored by Transitions at ISOP 2019	Kristin Klaue (Hecht)
Polydays 2019 Poster Award	Dragos Mutruc (Hecht)
Physik-Studienpreis 2019 der Physikalischen Gesellschaft zu Berlin	Laura Orphal-Kobin (Benson/ Schröder)
Royal Society of Chemistry Poster Prize (2019)	Valentin Reiter-Scherer (Rabe)
ERC Starting Grant (2019)	Tim Schröder (Schröder)
Brain Pool Award, Korean National Research Association (2019)	Matthias Staudacher
Quantum Futur Award 2019	Aron Vanselow (Ramelow)
2019 Chinese Government Award for Outstanding Self-financed Students Abroad	Fengshuo Zu (KochN)

8. LIST OF ABBREVIATIONS

- AFI Max Planck Institute for Gravitational Physics (Albert Einstein Institute)
- Work association of German University Professors ADUC for Chemistry (Arbeitsgemeinschaft Deutscher Universitätsprofessoren und -professorinnen für Chemie)
- Austrian Institute of Technology AIT
- AvH Alexander von Humboldt Foundation
- BAM Federal Institute for Materials Research and Testing (Bundesanstalt für Materialforschung und prüfung)
- BMBF German Federal Ministry for Science and Research (Bundesministerium für Bildung und Forschung)
- BMS Berlin Mathematical School
- Berlin University Alliance BUA
- Berlin Research 50 BR 50
- Chinese Academy of Sciences CAS
- Chiba U Chiba University
- French National Centre for Scientific Research CNRS (Centre national de la recherche scientifique)
- COST European Cooperation in Science and Technology
- CRC Collaborative Research Centre

German Academic Exchange Service German Science Foundation DFG DWI - Leibniz-Institut für Interaktive Materialien DWI FCRC Experimental and Clinical Research Centre ERC European Research Council ETH Zürich Eidgenössische Technische Hochschule Zürich EPFL École Polytechnique Fédérale de Lausanne Findable, Accessible, Interoperable, and Reusable FAIR FAIR-DI FAIR Data Infrastructure for Physics, Chemistry, Materials Science. and Astronomy e.V Ferdinand-Braun-Institut, Leibniz-Institut für FBH Höchstfrequenztechnik FHI Fritz Haber Institute of the Max Planck Society Frankfurt Institute of Advanced Sciences FIAS FMP Leibniz Forschungsinstitut für Molekulare Pharmakologie FU Berlin Freie Universität Berlin GenFab Generative manufacturing processes for hybrid components

DAAD

- GDCh German Chemical Society (Gesellschaft Deutscher Chemiker)
- HIOS Hybrid Inorganic/Organic Systems for Opto-Electronics
- HHI Fraunhofer Institute for Telecommunications, Heinrich Hertz Institute
- HU Humboldt-Universität zu Berlin
- HZB Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
- IAP Fraunhofer Institute for Applied Polymer Research
- ICMAT Institute of Mathematical Sciences
- IMPRS International Max Planck Research School
- INAM Innovation Network for Advanced Materials
- IKZ Leibniz Institute for Crystal Growth (Leibniz-Institut für Kristallzüchtung)
- IOP Institute of Physics
- IRI Integrative Research Institute
- **IRIS** Adlershof
 - Integrative Research Institute for the Sciences Adlershof
- IRTG International Research Training Group
- ISOP International Symposium on Photochromism
- JLSR Joint Laboratory for Structural Research
- KMPB Kolleg Mathematik und Physik Berlin

- MBI Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy
- MITP Mainz Institute for Theoretical Physics
- MPG Max Planck Society (Max-Planck-Gesellschaft)
- MPI-CEC Max Planck Institute for Chemical Energy Conversion
- MPI-KG Max Planck Institute of Colloids and Interfaces (Max-Planck-Institut für Kolloid- und Grenzflächenforschung)
- MPI-P Max Planck Institute for Polymer Research
- NBI Niels Bohr Institute
- NUS National University of Singapore
- NOMAD Lab

Novel Materials Discovery Laboratory

- PDI Paul-Drude-Institut für Festkörperelektronik
- PI Principal Investigator

Princeton U

Princeton University

- RTG Research Training Group
- RWTH Rheinisch-Westfälische Technische Hochschule Aachen
- SALSA School of Analytical Sciences Adlershof
- SOURCE Resources Center
- TFT thin film transistor

TU BerlinTechnische Universität Berlin

8. List of Abbreviations

UHV ultra-high vacuum

UNICAT Cluster of Excellence "Unifying Concepts in Catalysis"

U Potsdam

Universität Potsdam

- WEF World Economic Forum
- WIAS Weierstrass Institute for Applied Analysis and Stochastic
- ZIB Zuse Institute Berlin

7.4. Awards, Academic Prizes, and Honors

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