

## IRIS Adlershof – Biennial Report 2021/2022





## PREFACE

IRIS Adlershof has strengthened its position as an internationally recognized and highly visible actor in the areas of *Hybrid systems* as well as *Space–Time–Matter*. Moreover, new research areas *Big Data*, *Quantum Technology* and *Catalysis* have been established. In all these areas, the members of IRIS Adlershof are significantly involved in the acquisition and establishment of new and large national collaborative projects.

Internationally, in addition to our long-term strategic partners *Princeton University* and the *National University of Singapore*, IRIS Adlershof has enhanced its co-operations with the *Institute of Physics* of the *Chinese Academy of Sciences* as well as with the *Pritzker School of Molecular Engineering* at the *University of Chicago*.



This gratifying development levered strong support, including the improvement of our spatial and technical infrastructure through the successful commissioning of the *IRIS Research Building* during the reporting period: About 2.500 m<sup>2</sup> of state-of-the-art laboratory space and 2.200 m<sup>2</sup> of office and common rooms are now additionally available for IRIS Adlershof and its scientific partners worldwide. A special highlight was the festive opening, which attracted large public attention.

Within its regular evaluation in 2021, the review panel of international scientists recognized this success and recommended that Humboldt University should extend IRIS Adlershof for an additional third period of three more years. Moreover, the panel recommended that the university shall take measures, suitable for continuing the two main research

areas IRIS Adlershof, *Hybrid systems* and *Space–Time–Matter*, in the long term.

In view of the fact that IRIS Adlershof has been founded as a temporary institution of Humboldt-Universität, we appreciate that we could anchor our two original main research fields in sustainable university structures: The research field of *Hybrid systems* has led to the establishment of a new Central Institute *Center for the Science of Materials Berlin* (CSMB) at Humboldt-Universität zu Berlin in September 2022. Furthermore, the research field *Space–Time–Matter*, was transferred to the *Kolleg Mathematik Physik Berlin*, an Interdisciplinary Center of Humboldt University.

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 cooperation.

Sincerely,



Prof. Jürgen P. Rabe  
Director



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# 1. Executive Summary

IRIS Adlershof looks back on two successful years with significant positive growth. In 2021 and 2022, the *Integrative Research Institute for the Sciences Adlershof* opened its own research building, established three new research areas and fortified the two main research areas. The latter, *Hybrid Systems* and *Space–Time–Matter*, have now both been transferred to sustainable university structures, the *Center for the Science of Materials Berlin* and the *Kolleg Mathematik Physik Berlin*. Due to an excellent evaluation, the Board of Governors of Humboldt Universität zu Berlin has extended IRIS Adlershof for its final period at another three years, until October 31, 2024.

## EXCELLENT SCIENTIFIC ACHIEVEMENTS

A clear indication of IRIS Adlershof's positioning in the scientific scene are the scientific achievements of its 35 members and over 200 early career researchers. Their work was presented to the international scientific community in high impact journals and at national and international conferences, largely held online.

Among the scientific highlights from 2020 is *Xolography for linear volumetric 3D printing*, published by IRIS member Stefan Hecht and his multidisciplinary team in *Nature*. One of the highlights from 2021 is *Classical Gravitational Bremsstrahlung from a Worldline Quantum Field Theory*, which was published by IRIS member

Jan Plefka and his group in the journal *Nature Communications*.

Major scientific highlights will be discussed in chapter two (pp. 37) of this report.

Altogether more than 400 peer-reviewed publications appeared in high impact journals. A list of selected publications can be found in the chapter 5 (pp. 81).

## SUCCESSFULL 2<sup>nd</sup> EVALUATION

Based on a self-report as well as videos, IRIS Adlershof presented itself to an international expert panel in an online visit on May 10–11, 2021, which included presentations of the achievements and plans as well as in-depth discussions with various groups of IRIS members and the university management.

The committee praised that all major goals and suggestions put forward by the review panel

in 2017 (internationalization, membership of junior group leaders, development of a long-term strategy) were fulfilled and partly exceeded.

In December 2021, the Board of Governors (Kuratorium) of Humboldt-Universität zu Berlin followed a corresponding proposal by the Academic Senate of the HU, which is based on the successful evaluation of IRIS Adlershof and decided to extend IRIS Adlershof until October 31, 2024. According to the constitution of the HU, the maximum duration of an Integrative Research Institute will then be reached.

While the research field *Space–Time–Matter* was already expanded and consolidated with the interdisciplinary center *Kolleg Mathematik Physik Berlin*, headed by Matthias Staudacher since 2021, a new central institute (Zentralinstitut) was founded in 2021 as recommended by evaluation committee to increase the expertise at

Campus Adlershof in the field *Materials Science*. Stefan Hecht was appointed back to Humboldt Universität as a professor and as the founding director of the *Center for the Science of Materials Berlin* in 2022.

## PROMOTION OF JUNIOR SCIENTISTS

Following the recommendation of the expert commission and with the aim of continuous further improvement, IRIS Adlershof significantly expanded its measures to support young scientists.

For example promising doctoral candidates can apply for an IRIS Adlershof fellowship:

With her thesis, Archana Manoharan helped to understand the electronic properties of  $\text{Cu}_2\text{ZnSnS}_4$ , which consists of earth abundant and non-toxic elements. This is a promising candidate as an absorber layer, i.e. the core of the

solar cell device to absorb sunlight and transport the resulting charge carriers to the electrical contacts. IRIS Adlershof supported this research with a fellowship, so Archana could finalize the project getting the results ready for publication.





In June 2022 the young scientists met and elected Laura Orphal-Kobin their representative in the IRIS bodies and Pablo Hernández López as her deputy. Thus, the young scientists are represented in the IRIS general meetings as well as in the IRIS Council with the right to speak, propose and vote. This step was necessary, since the previous representative Julian Miczajka has

started his postdoctoral career at the Max-Planck-Institute for Physics in Munich and his deputy Sven Ramelow became a full member of IRIS Adlershof.

Laura Orphal-Kobin is a PhD student in the group of Tim Schröder within the graduate school *Berlin School of Optical Sciences and Quantum Technologies* and is doing research on the optimization of diamond nanostructures.

Pablo Hernández López is a PhD student in the group of Sebastian Heeg and is carrying out research on one- and two-dimensional new materials. He is a member of the graduate school *Advanced Materials*.

Supported by the IRIS branch office they initiated an ongoing series of event (see p. 12).

## NEW IRIS MEMBERS

Since the recruitment of new highly qualified scientists as members is of utmost importance for outstanding research results and for the further growth of a research institute, it should be emphasized that IRIS Adlershof gained ten new members in the reporting period.

Morover six promising researchers joined as a new junior members in 2021. To increase their visibility and reflect their importance all eight junior members, the six mentioned below plus Michael J. Bojdys and Valentina Forini, received full membership with the update of the statute in 2022:

*Stijn van Tongeren* is leading an Emmy-Noether Independent Junior Research Group at the Department of Physics of HU since fall 2018 and became IRIS junior member in March



2021. He and his group work towards integrable deformations of AdS/CFT and related holographic structures. This research is expected to uncover novel insights into the structure of quantum field theories and their dual string theories. His work is thus closely connected to that of the IRIS members Matthias Staudacher and Jan Plefka. Van Tongeren's junior research group receives more than one million Euros in funding over six years by DFG. Since 2020 he is also PI in RTG 2575 *Rethinking Quantum Field Theory*.

*Oliver Dumele* joined Humboldt-Universität zu Berlin in 2019 as leader of the independent research group, funded by a Liebig scholarship. His current research focuses on the design and synthesis of supramolecular materials, photomagnetic molecular switches, and covalent organic frameworks (COFs) with applications in sensing and battery materials.



*Nichol Furey* is a 'Freigeist' fellow of the Volkswagen Foundation at the Department of Physics at HU and at IRIS Adlershof. She researches the algebraic structure of elementary particle physics as well as octonions and the standard model of particle physics.





Since August 2020 *Emanuel Malek* is leading an Emmy-Noether Independent Junior Research Group on “*Exploring the landscape of string theory flux vacua using exceptional field theory*”

at the Physics Department of Humboldt-Universität zu Berlin, where he also closely collaborates with the IRIS-groups of Jan Plefka, Matthias Staudacher and Olaf Hohm. Malek's Junior Research Group will receive more than 1.2 M€ in funding over 6 years from the German Research Foundation. After finishing his doctoral studies at the University of Cambridge in 2014, Malek spent one year as a Postdoctoral Fellow at the University of Cape Town, followed by a three-year-long stay as a Research Fellow at the

Ludwig Maximilian University Munich. He subsequently worked at the Max-Planck-Institute for Gravitational Physics in Potsdam for two years.

*Sebastian Heeg* heads an Emmy Noether junior research group at the Department of Physics at HU. He is interested in the investigation of low-dimensional solid-state systems, for example graphenes and nanotubes, employing optical spectroscopy.





Since 2019, *Markus Krutzik* is leading the „Joint Lab Integrated Quantum Sensors“ at the Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenz-

technik, where he has already been working as a guest researcher since 2017. Additionally, he has been a group leader at Humboldt-Universität zu Berlin since 2015, working on Quantum Sensors and Optical Technologies for Space Applications. His research focuses on the development of the next generation of chip-scale quantum sensors for real world applications. Krutzik finished his doctoral studies at Humboldt-Universität zu Berlin in 2014. He then worked as a Postdoctoral researcher at the Cold Atom Laboratory of

NASA's Jet Propulsion Laboratory between 2014 and 2015, where he continued to work as a Technical Consultant between 2016 and 2018.

Besides, the following successful scientists were directly admitted with a full membership:

*Eva Unger* has received a professorship at the Department of Chemistry at HU in 2022. She is also head of the department "Solution processes for hybrid materials and components" at the Helmholtz-Zentrum Berlin and has already been working closely with IRIS Adlershof as part of the Joint Lab *GenFab* before





her membership. In particular, she is interested in scalable deposition methods of high value semiconductors such as metal halide perovskites and a deeper understanding of layer formation.

The Materials scientist and theoretical physicist *Matthias Scheffler*, head of the NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society and honorary professor at the Department of Physics at the HU, conducts research on fundamental aspects of the chemical and physical properties of surfaces as well as on methodological developments in artificial intelligence to solve fundamental problems



in materials science. Since 2020, he leads the European Center of Excellence NOMAD together with Claudia Draxl, who is also a member of IRIS Adlershof, and is Co-speaker of the NFDI consortium FAIRmat.

The physicist *Julia Stähler* is a professor at the Department of Chemistry at the HU with a research focus on ultrafast spectroscopy on nanostructured materials, in particular also on inorganic/organic hybrid systems. She is a subproject leader in the Collaborative Research Center 951 *Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS)*, one of the lighthouse projects of IRIS Adlershof.





Also *Ulf Leser* became a member of IRIS Adlershof in the end of 2021. He is a full professor at the Department of Computer Science at Humboldt-Universität zu Berlin. His main research interests are biomedical data management and text mining, infrastructures for large-scale scientific data analysis, and statistical Bioinformatics. He is speaker of the CRC "Foundations of Workflows for Large-Scale Scientific Data Analysis (FONDA)" and of the collaborative research project "Comprehensive Data Integration for Precision Oncology".

With their expertise, these new members will contribute immensely to the further expansion and interlinking of the IRIS research areas and thus strengthen the Institute itself. IRIS Adlershof is very pleased about this enrichment.

In order to increase the visibility of our junior members and to reflect their importance for the scientific life of IRIS Adlershof, the distinction between full and junior members, which was originally defined in the IRIS statutes, has been abolished at the end of 2022 on the recommendation of the review committee. Thus, all previous junior members are now equal members of IRIS Adlershof with equal rights and duties

During the reporting period, two members left IRIS Adlershof to pursue different scientific activities: *Jochen Brüning* and *Alexander Reinefeld*, both IRIS Adlershof's founding members, left the Integrative Institute for the Sciences in 2021. IRIS Adlershof would like to express its

appreciation for the excellent and fruitful cooperation over the years!

A list of all current members of IRIS Adlershof can be found in chapter 3.3 (pp. 68).

makes it a symbol of the continuous spatial and scientific growth of IRIS Adlershof. Details on the research infrastructure are presented in chapter 3.4 (pp. 73).

## OPENING OF THE RESEARCH BUILDING

With regard to IRIS Adlershof's goal of creating the best possible framework for cutting-edge research, the opening in October 2022 was a milestone event for IRIS Adlershof.

The IRIS research building provides outstanding scientists with excellent working conditions, allows the IRIS research areas to expand and it will further strengthen IRIS Adlershof's international appreciation. This



## NEW COOPERATION PROJECTS

Due to its unique architecture as an Integrative Research Institute, IRIS Adlershof is an attractive partner for pertinent non-university institutions and innovative enterprises. In addition to a large number of cooperations via its members, IRIS Adlershof has started several cooperations in the reporting period. The most important new projects in the past two years are the joint catalysis research laboratory with Helmholtz-Zentrum Berlin (HZB) *CatLab* and the incubator programme *AdMaLab* with the *Innovation Network for Advanced Materials e.V* (INAM) and various start-ups.

In early 2021, HZB and Humboldt-Universität zu Berlin signed a cooperation agreement, aiming to establish a joint research laboratory for catalysis in HU's IRIS research building in Adlershof. This meanwhile operating laboratory is part of the *CatLab* research

platform funded by the German government, which HZB operates jointly with the Fritz Haber Institute and the Institute for Chemical Energy Conversion of the Max Planck Society.

In this context part of the IRIS laboratories in Berlin-Adlershof have been equipped for the development and investigation of heterogeneous catalyst systems. In an open-plan laboratory reactors have been installed to determine the catalytic activity and selectivity of the material 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 are used, which are completed by the high-end analysis options of the neighbouring synchrotron radiation source BESSY II of the HZB. We also cooperate closely in the field of thin-film technology, using additive



manufacturing processes and nano-structuring and synthesis methods.

In spring 2022 representatives of the Innovation Network for Advanced Materials (*INAM e.V.*) and Humboldt-Universität zu Berlin welcomed numerous guests from business, politics, research and teaching to the opening event of the incubator programme *AdMaLab - The Berlin Materials and Hardware Lab* in the research building of IRIS Adlershof at Humboldt-Universität.

As part of the *Berlin Startup Stipendium* funding programme, the Berlin Senate Department for Economics, Energy and Public Enterprises has provided INAM e.V. and its cooperation partners with around 1.1 million euros to set up an incubator programme tailored to material science start-ups.

AdMaLab provides:

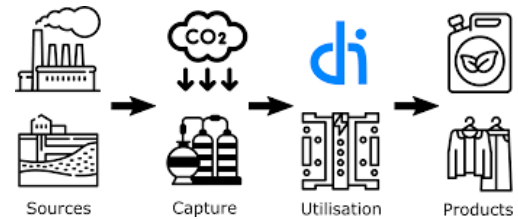
- » a stipend of 2,200 EUR / month for 12 months
- » Guided access to a lab space at the newly opened research building of the IRIS Adlershof at Humboldt University and to the HySPRINT Innovation Lab at the Helmholtz-Zentrum Berlin
- » co-working spaces in Berlin Mitte and Adlershof
- » training on IP strategy, investment and funding opportunities, business strategy, finance, setting up and running a company, investor readiness,
- » technical & business mentoring supported by Humboldt Innovation GmbH and experts from various specialist areas
- » pitch training and networking

A jury from business and academia selects Berlin-based individual innovators and early stage start-ups (less than 3 months old) with a convincing idea and a developed plan. They join our intensive AdMaLab programme and learn how to take their innovative technologies to the next level.

IRIS Adlershof is working together with the following start-ups in the research building:



*Meloon* filters environmentally harmful carbon dioxide from flue gas and produces Graphene from it as a raw material. Consequently, CO<sub>2</sub> is removed and stored long-term in the form of Graphene and other solutions. Meloon uses the Graphene to manufacture its filtrating membranes, which represents a profitable solution to CO<sub>2</sub> sequestration.



The world is facing the challenge of finding alternatives to fossil fuels. However, tomorrow's circular carbon economy is fundamentally limited by the inefficient catalysts available today.

*Dunia Innovations* aims to overcome this the bottleneck to scalable carbon utilization by building the world's first self-driving lab for carbon dioxide utilisation catalysis. By leveraging the 21<sup>st</sup> century AI and robotic tools, *Dunia Innovations* supercharges the catalyst innovation process and reduces time and cost to market in this area by up to 90%.

Surface enhanced Raman spectroscopy (SERS) is a powerful vibrational spectroscopy technique that allows for highly sensitive structural detection of low concentration analytes.



*MetaMem* has developed an improved manufacturing process to overcome limited surface enhancement associated with Raman spectroscopy. Their scalable and optimized pathway to create porous metal membranes allows them to find applications in fields where SERS has not been available yet, while also tapping into the already existing SERS market.



In spite of recent advancements, there is no a commercial solution for high-capacity electrode materials in rechargeable batteries that is truly flexible and heat resistant.

*Mana.energy's* products enable the emergence of fundamentally novel battery-powered products for which conventional batteries are not a viable alternative.



The start of the *FAIRmat* in 2021 is an example of a new successful transnational cooperation project.

*FAIRmat* (FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids) is part of the National Research Data Infrastructure (NFDI). The NFDI is a nationwide network currently being established and funded by the federal and state governments with up to 90 million € per year from 2019 to 2028 to systematically manage research data.

*FAIRmat* represents the diverse research field of the Condensed Matter Section of the German Physical Society (DPG) as well as the chemical physics of solids. The project receives funding to build an infrastructure that will make materials science data FAIR: findable, accessible, interoperable, and re-purposable. This will enable researchers in Germany and beyond to store, share, find, and analyze data over the long term.



*FAIRmat* is led by IRIS member Claudia Draxl. She looks back on the project start with satisfaction: "We were able to welcome 30 dedicated new staff members and move into our new headquarters in IRIS Research building is imminent. We were already able to realize a first large colloquium with the renowned FAIR data expert Barend Mons and a total of 130 online and offline participants. Both the application and the successful project start would not have been possible without the support of IRIS Adlershof."

*FAIRmat* will run for five years in the first phase. A total of 60 project leaders from 34 German institutions will work together, including Cristoph T. Koch and Matthias Scheffler who are members of IRIS Adlershof. In addition to HU Berlin, the Leibniz Institute for Crystal Growth (IKZ), the Max Planck Institute for Chemical Energy Conversion (MPI CEC), the Fritz Haber Institute of the Max Planck Society (FHI), the Technical University of Munich (TUM), the

Karlsruhe Institute of Technology (KIT) and the non-profit association FAIR-DI e.V. are also involved in the project as co-applicants.

## INTERNATIONAL VISIBILITY

In order to strengthen its visibility in the two current IRIS research areas and to further profile the Adlershof campus as a place of international innovative research, IRIS Adlershof initiated new and intensified existing fruitful cooperation with international partner institutions that are world leaders in those research areas during the reporting period.

Particularly noteworthy is the scientific cooperation between IRIS Adlershof and the *Institute of Physics (IOP)* of the *Chinese Academy of Sciences (CAS)*. The partnership started with joint workshops and delegation visits. The most visible result of this international cooperation between the IOP and IRIS Adlershof so far is a joint postdoc 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 Zhongguancun Beijing Campus and one year in

HU's natural science campus in Berlin 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 are financially supported by up to 4,500 EUR/month. While the first round of applications began in early 2021, due to strict corona regulations, the first visa was not issued to a grantee until late 2022. We hope to welcome Jing Ming from IOP-CAS to IRIS Adlershof in the near future.





Another successful cooperation began in November 2021 with the visit of four scientists of the *Pritzker School of Molecular Engineering* at *University of Chicago* at IRIS Adlershof.

Due to the scientific and strategic proximity of the two institutes, a research collaboration program was initiated, including the set up of an annual Summer School program.

## SCIENTIFIC EVENTS

In order to not only communicate its member's ground breaking scientific results to the international professional public, to promote its young scientists and to strengthen and expand its national and international visibility and cooperation, but also to present the institute and

the cutting-edge research conducted here to a broader audience, several scientific events were held during the reporting period. Many events have been organized by our members, who always got full support by the branch office if needed, e.g. seminars, symposia and workshops.

We would like to point out the following events organized by IRIS Adlershof as a whole.

*IRIS Colloquia* are an important open event to bring all members and junior scientists together and discuss scientific progress.

In March 2021 an IRIS Colloquium was held with Stijn van Tongeren on "Exactly solvable models and holography", Emanuel Malek on "Listening to the shape of string theory's extra dimensions" and Markus Krutzik on "Atomic systems for timing and sensing applications".

In the next colloquium in October 2021 Sebastian Heeg gave a talk on "Exploring Confined Carbyne", followed by the talks of



Oliver Dumele on "Novel Topologies in Covalent Organic Framework Chemistry" and Ulf Leser on "CRC 1404 FONDA - Foundations of Workflows for Large-Scale Scientific Data Analysis" in November.

In July 2022 the speaker Prof. Dr. Ilia Solov'yov gave a talk on "Modelling of dynamical processes in molecular systems with stochastic dynamics", followed in August with an talk on "Engineering nanodiamond quantum sensors for practical applications" by speaker Prof. Masazumi Fujiwara (Okayama U, Japan).

The first summer school together with the Pritzker School of Molecular Engineering (University of Chicago) was organized by IRIS Adlershof and carried out in summer 2022 at HU's science campus in Adlershof: *Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and*

### *Artificial Intelligence - A Workshop and Hands-on Tutorial.*

During the first three days from July 25<sup>th</sup> to 27<sup>th</sup>, leading experts from various fields gave talks on computational applications and related artificial intelligence methods in relation to advances in materials science. On the first two evenings, there were dinners with poster sessions for further scientific and collective exchange. The afternoon of July 27<sup>th</sup> was followed by an excursion to a graffiti tour at Teufelsberg followed by dinner.

The last two days were then used for tutorials with hands-on examples focusing on the simulation of molecular dynamics.

### SOCIAL EVENTS

For an interdisciplinary institute like ours, the corona pandemic since 2020 was a great challenge, as it severely limited the lively exchange and active life on campus. Therefore, it was important to bring our people together again with low-threshold events, as far as low infection numbers allowed.

We held an outdoor barbecue in the summer of 2021 and a summer party in 2022 together with the Department of Physics.

IRIS Adlerhof was aware of its responsibility and had a strict hygiene concept for both events, coordinated with experts from the HU, in order to minimise the residual risk. No corona infections are known from either event.

With the relaxation of the Corona measures, the low numbers and the increased immunity,



indoor activities were also possible in good conscience at the end of December 2022.

On Nov 21<sup>st</sup>, 2022 the IRIS junior scientists met for a breakfast and a lab tours session focused on quantum optics. Pablo Hernández López, the juniors representative and organizer, explains: "Our colleagues Elisa & Martin (Krutzik group) and Julian & Jonas (Schröder group) showed their labs and introduced their fields of research. This event was the first one of a series of lab tours that will continue next year. Thanks to the presenters and to everyone who came. It was great to meet so many new colleagues and to discover some of the very interesting work done at IRIS Adlershof."

On the December 13<sup>th</sup>, 2022, the young researchers of IRIS Adlershof convened for a momentous Christmas celebration. The event took place in a common room within the research building, and was not merely a casual social gathering, but rather a solemn occasion

for the participants to deepen their knowledge of science and technology. To this end, they engaged in a challenging scientific quiz that tested their knowledge of various topics related to the holiday season, which led to numerous enlightening discussions, and shared their love of science with their colleagues and friends.

## GENDER EQUALITY

IRIS Adlershof sees itself as a place of diversity, plurality of opinion, mutual appreciation, and respect. Therefore, IRIS Adlershof is attaching great importance to the provision of equal opportunities. 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 doctoral candidate Archana Manoharan was actively supported in taking the next step in their academic careers through interim financing and scholarships, that enabled her to begin, as well as successfully complete, her doctorates and to publish her results. Three female IRIS junior research group leaders – Catherina Cocchi, Valentina Forini, Yan Lu – accepted external calls for permanent academic positions, reflecting the attractiveness of our members, but challenges IRIS Adlershof to engage more women at the campus again.

## FUTURE GOALS

For the next and last reporting period, we are planning further growth and thematic development of IRIS Adlershof. We have set ourselves the following goals:

Future plans concern both, the continuation of running projects, initiated during the previous funding periods, as well as new projects, with impact way beyond the upcoming funding period.

The early flagship project of IRIS Adlershof, CRC 951 *Hybrid Inorganic/Organic Systems for Optoelectronics* (spokesperson N. Koch, with further eight members of IRIS Adlershof as principal investigators) will expire in 2023, laying the ground for a new CRC initiative.

With the IRIS Research Building in full operation, advantage will be taken of its considerable new opportunities through the *Joint Lab for Generative manufacturing processes for hybrid components (GenFab)*, and the *Joint Lab for Microscopy*. Beyond this, the *Joint Lab for Microscopy* aims to develop into a Berlin-wide core facility, the *IRIS Microscopy Center* aligned with the fifth objective of the BUA *Sharing Resources*. It features already a broad range of

state-of-the-art electron microscopy facilities, including – at the high end – a NION-TEM with a unique combination of extremely high spatial and spectral resolution.

The development of a concept towards a Cluster of Excellence in the Excellence Strategy is one of the major goals for the upcoming funding period of IRIS Adlershof.

Parallel, we will establish the newly founded *Center for the Science of Materials Berlin* (CSMB) as a functional and effective central institute of the HU – a sustainable outcome of the IRIS research field *Hybrid Materials*.

Members of IRIS Adlershof are also already participating in and contributing to three Clusters of Excellence, all funded until the end of 2025 and they can be continued pending successful re-evaluation. Activities in the IRIS research area *Mathematical Physics of Space–Time–Matter* will be sustained beyond the upcoming funding

period of IRIS Adlershof by developments within the *Kolleg Mathematik und Physik Berlin*.

To further support early career researchers, a proposal for a Research Training Group (a funding line of the DFG) related to the proposal of a new Cluster of Excellence will be submitted.

Likewise, the support of junior faculty is essential to achieve our overarching goals and will be further enhanced, particularly through the opportunities provided by the IRIS Research Building. Major efforts will be devoted to increase the number of females yet again, since three female IRIS junior research group leaders – Caterina Cocchi, Valentina Forini, Yan Lu – accepted external calls for permanent academic positions.

All research areas will leverage the attractiveness of Berlin as a hub for start-ups. As a co-founder of the *Innovation Network for Advanced Materials* in Berlin, and as a direct supporter of start-ups, such as the Adlershof-based

*INURU GmbH* and the recently founded *xolo GmbH*, IRIS Adlershof can build on solid fundamentals.

As a new instrument for internationalization, a two-year Postdoctoral Fellowship Program was established in the current IRIS funding period between IRIS Adlershof and the Institute of Physics (IOP) of the Chinese Academy of Sciences (CAS). This prestigious fellowship program will be continued and expanded in the upcoming IRIS funding period.



## 2. Scientific Highlights

Scientific results are regularly presented by IRIS Adlershof on its website ([www.iris-adlershof.de](http://www.iris-adlershof.de)). In order to communicate the achievements of its members not only to the international professional public, but also to interested readers without detailed expertise in the fields being

discussed, a generally understandable presentation method was chosen.

These are the scientific highlights of 2021 and 2022:

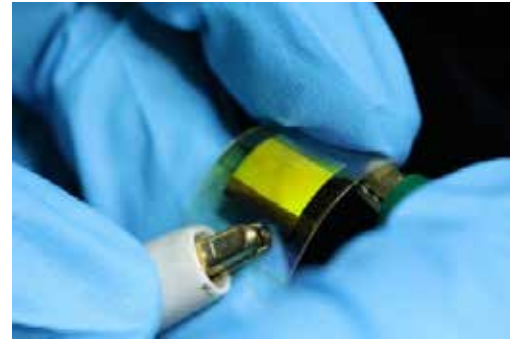
### INKJET-PRINTED ELECTRODES IN OLEDs (ORGANIC LIGHT-EMITTING DIODES)

Researchers in the HySPRINT joint lab *Generative Manufacturing Processes for Hybrid Components (GenFab)* of Humboldt-Universität zu Berlin and Helmholtz-Zentrum Berlin have successfully implemented an ink produced by the Berlin-based company OreITech in solution-processed organic light emitting diodes.

After inkjet printing the particle-free silver ink, an argon plasma is used to reduce the silver

ions in the ink to metallic silver. “Because this process takes place at a low temperature, it is suitable for use with temperature-sensitive substrates, such as flexible plastic foils,” explains Dr. Konstantin Livanov, co-founder and CTO of OreITech. The researchers fabricated organic light-emitting diodes employing the silver ink as a transparent conductive electrode on the flexible substrate PET. The resulting devices show

comparable light output characteristics to those based on the otherwise widely used indium tin oxide (ITO). Crucially, however, the silver electrodes showed superior stability to ITO upon mechanical bending. Felix Hermerschmidt, senior researcher in the joint lab of HU and HZB, confirms, "The OLEDs based on the OrelTech ink remain intact at a bending radius at which the OLEDs based on ITO show breakage and fail." This opens up several application opportunities of the printed devices. The work has been published in the journal *Flexible and Printed Electronics* and is available Open Access. GenFab, led by Prof. List-Kratochvil, who is a member of IRIS Adlershof, is moving into laboratories and offices in the new IRIS research building for further research and development work.



The OLEDs incorporating the OrelTech ink illuminating under strain.

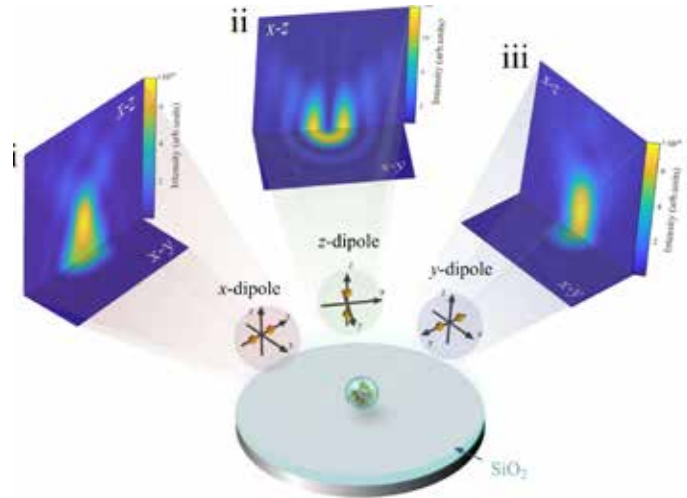
**ITO-free OLEDs utilizing inkjet-printed and low temperature plasma-sintered Ag electrodes**

M. Hengge, K. Livanov, N. Zamoshchik, F. Hermerschmidt, and E.J.W. List-Kratochvil  
*Flex. Print. Electron.*, 2021, 6, 015009.

DOI: 10.1088/2058-8585/abe604

## REAL-TIME OPTICAL DISTANCE SENSING OF UP-CONVERSION NANOPARTICLES WITH A PRECISION OF 2.8 NANOMETERS

Sub-diffraction limited localization of fluorescent emitters is a major goal of microscopy imaging. It is of key importance for so-called super-resolution, a technique that was awarded the Nobel Prize in Chemistry in 2014. A cooperation of researchers in Australia, China, the USA and IRIS Adlershof have now demonstrated ultra-precise localization and tracking of fluorescent nanoparticles dispersed on a mirror. The many randomly oriented molecular dipoles in such up-conversion nanoparticles (UCNPs) interfere with their own mirror images and create unique, bright and position-sensitive patterns in the spatial domain.



Calculated self-interference of a single nanoparticle placed on a mirror substrate with a silica layer as the spacer. (i), (ii) and (iii) show different cuts through the far-field patterns of oriented dipoles oscillating along the x, y and z-axis, respectively.

The pattern can be detected in the far-field by a sensitive camera and was compared to a detailed and quantitative numerical simulation. In this way it was possible to localize individual particles with an accuracy of only 2.8 nm, a value which is smaller than  $1/350$  of the excitation wavelength.

The localization can be performed rapidly, and a single particle can be followed with a 50Hz frame rate. This is much faster than other self-interference-based methods based on mapping of the fluorescence spectrum. A special benefit of UCNPs is their high photo-stability

and sensitivity, e.g. to temperature and PH. Therefore, the novel technique may be used for high-resolution multimodality single-particle tracking and sensing.

### **Axial Localization and Tracking of Self-interference Nanoparticles by Lateral Point Spread Functions**

Y. Liu, Z. Zhou, F. Wang, G. Kewes, S. Wen, S. Burger, M. Ebrahimi Wakiani, P. Xi, J. Yang, X. Yang, O. Benson, and D. Jin  
*Nat. Commun.*, 2021, 12(1), 2019.  
DOI: 10.1038/s41467-021-22283-0

### **A RAY OF HOPE FOR QUANTUM RESEARCH - DIRECTLY MEASURING THE PARTICLE EXCHANGE PHASE OF PHOTONS**

A research team from Humboldt-Universität zu Berlin and partners have for the first time directly measured the particle exchange phase

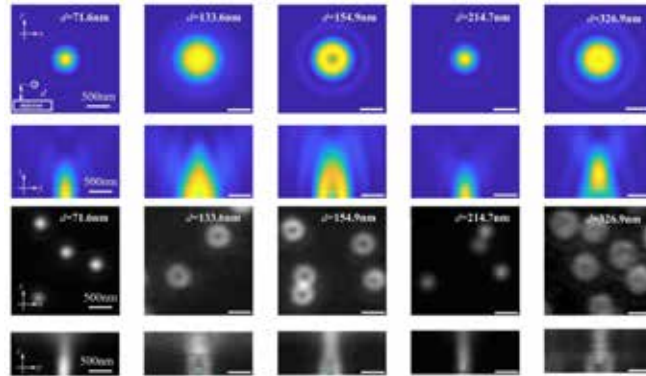
of photons. This experiment provides direct evidence for an astonishing quantum phenomenon that is only observed in completely similar



quantum objects. This represents an important step forward in quantum research.

The particles the research team is on the trail of are elusive. The physicists are investigating the quantum particles of electromagnetic waves, also called photons, which make up light. Photons can only be distinguished if they have different wavelengths, oscillate in different directions or are located at different points in space and time.

"If two photons that are indistinguishable in wavelength and direction of oscillation meet and separate again, they have in a sense lost their identity," explains Kurt Busch. "Imagine we send two twins through two doors into one room. When they step out again, we cannot determine whether they each used the same door to do so or not," adds Oliver Benson, a member of IRIS



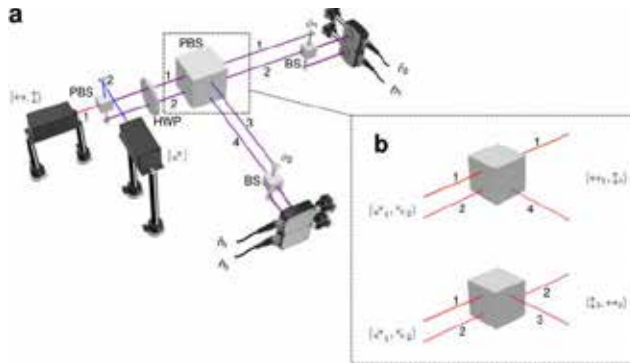
Simulated (topmost two rows) and experimental (bottommost two rows) far-field self-interference emission patterns. The particle-to-mirror distance increases from the left to the right column from 72nm to 327nm. All scale bars are 500 nm.

Adlershof. Nevertheless, something happens in quantum mechanics. According to the so-called symmetrisation postulate, there are two categories of elementary particles: Bosons and fermions. These types of particles differ in what happens when you swap them with each other.

In the example, this would mean that each of the twins leaves the room through the other door. In the case of bosons, nothing changes - in the case of fermions, the quantum mechanical wave function describing the particles receives a phase shift, which is also called the exchange phase. "In the twin example, you can perhaps think of it like this: If we send the two twins into the room in step and they come out of different doors, they continue to be in step. As bosons, the twins step out of the room with the same leg in front that they first used to step into the room. However, as fermions, they both need one more step and now walk with the other leg when leaving the room," says Benson. "That photons are bosonic could previously only be shown by indirect measurements and mathematical calculations," says Kurt Busch. "In our latest experiment, we have directly measured the particle exchange phase of photons for the first

time, providing direct evidence for their bosonic character."

To directly demonstrate the exchange symmetry of a state for two identical particles, the team set up an optical apparatus with an interferometer. At the heart of the setup - the size of a small table - are two beam splitters. Two photons were then sent into the interferometer and guided through the beam splitter along two different paths. Along one of the two paths, the photons are interchanged with each other, while along the other they remain unchanged. At the exit of the interferometer, both photons were then superimposed again at the second beam splitter. "Depending on whether the photons are bosonic or fermionic, the two photons are then in step and amplify each other, or they are out of step and cancel each other out," the physicists explain.



Conceptual sketch of the interferometer setup:

a: An entangled photon pair (red beam) is fed into the interferometer, which produces two different possibilities at the central polarising beam splitter (PBS), as shown in

b: Either the photon in path 1 is transmitted and the photon in path 2 is reflected, or exactly the opposite. The quantum superposition of these scenarios leads to the interference between states that are physically reversed versions of each other, revealing the particle exchange phase  $\phi_x$ . The blue beam is generated by an attenuated laser and serves as a reference signal to determine the effective optical path length differences,  $\phi_{-1}$  and  $\phi_{-2}$ .

Future improvements to the interferometer will provide a new tool for precision measurements with quantum light. At the same time, the experiment establishes a new method for generating and certifying quantum states of light. This is very important in the new field of quantum information processing, on the basis of which novel, much more powerful computers are currently being developed.

### Direct observation of the particle exchange phase of photons

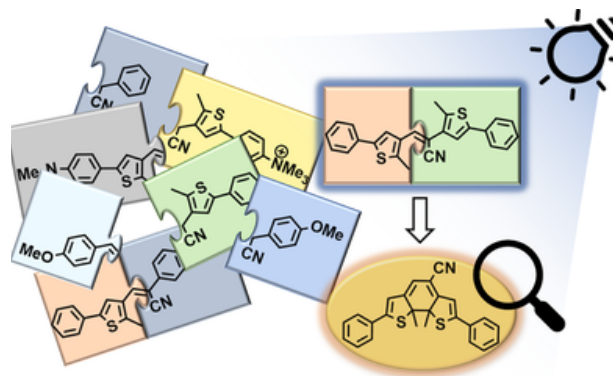
K. Tschernig, C. Müller, M. Smoor, T. Kroh, J. Wolters, O. Benson, K. Busch, and A. Perez-Leija

*Nat. Photonics*, 2021, 15(9), 671.

DOI: 10.1038/s41566-021-00818-7

## FISHING WITH LIGHT - ACCELERATED DISCOVERY OF $\alpha$ -CYANODIARYLETHENE PHOTOSWITCHES

Molecules are usually optimized for a task by trial and error. Time-consuming iterative rounds of synthesis and characterization provide detailed insight into structure-property relationships. In order to speed up this tedious process, Niklas König and Dragos Mutruc from the HechtLab have developed a clever means to generate an equilibrating mixture, a so called dynamic constitutional library, of photoswitchable molecules and used their wavelength-specific response to select the proper candidate. Thus, they could “fish” the desired switch with light in a pool of many different switches. The method should facilitate the rapid exploration of structural diversity in functional dye chemistry.



### Accelerated Discovery of $\alpha$ -Cyanodiarylethene Photoswitches

N. F. König, D. Mutruc, and S. Hecht  
*Journal of the American Chemical Society*, 2021,  
143(24), 9162.  
DOI: 10.1021/jacs.1c03631F

## SHAPING 2D MATERIALS WITH SMALL MOLECULES

Electronic properties of 2D materials such as graphene and transition metal chalcogenides can be tailored by shaping their topography at the nanoscale. At IRIS Adlershof, Abdul Rauf and colleagues from the RabeLab together with Igor Sokolov investigated how to shape surfaces and interfaces of 2D materials with small molecules, intercalating at the interfaces between the 2D materials and a solid substrate. Particularly, they investigated wetting of interfaces between graphene and a hydrophilic substrate, mica, with two small molecules, water and ethanol. Wetting with water leads to labyrinthine structures exhibiting branch widths down to the 10 nm scale. This is explained by a process leading to an equilibrium between electrostatic repulsion of the polar molecules preferentially oriented at the interface, and the line tension between wetted and non-wetted areas. Increasing line tension or

decreasing dipole density increases the branch width, causing eventually non-structured wetting layers. The method might be used to shape 2D materials to tailor their electronic properties.

### **Shaping surfaces and interfaces of 2D materials on mica with intercalating water and ethanol**

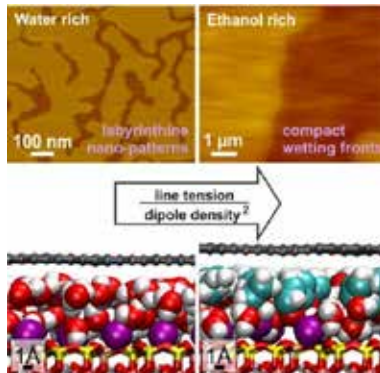
A. Rauf, J. D. Cojal González, A. Balkan, N. Severin, I. M. Sokolov, and J. P. Rabe  
*Molecular Physics*, 2021, 119(15-16), e1947534  
DOI: 10.1080/00268976.2021.1947534

## SPARKING ELECTROLUMINESCENCE IN POLY(TRIAZINE IMIDE) FILMS

A team of researchers from King's College London, Humboldt-Universität zu Berlin, Carl von Ossietzky Universität Oldenburg, and Helmholtz-Zentrum Berlin (HZB) have investigated the synthesis, structure, optical properties of poly(triazine imide), a member of the family of graphitic carbon nitrides. Their progress on

material quality and processing allowed for construction of the first single layer, organic light emitting device (OLED) with a solution-processed graphitic organic material as a metal-free emission layer.

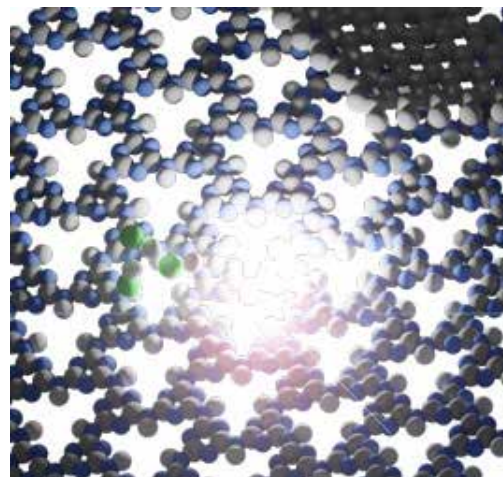
Organic semiconductors have sparked great interest in academic and industrial circles over the last decades, because of their advantageous properties such as (i) a high absorption coefficient compared to conventionally used silicon as well as (ii) less energy intensive production, and (iii) composition from earth-abundant elements. Progress in this field of research promises new,



Scanning force microscopy images of graphene surfaces shaped by an intercalating molecularly thin water layer self-assembled into labyrinthine patterns (top left), and the compact wetting front of an ethanol layer (top right). The snapshots of Molecular Dynamics simulations of the interfaces filled with molecules (bottom) helped to understand the origin of the forces driving the pattern formation.

cost- and energy-efficient technologies in consumer electronics, smart packaging, and flexible light-emitters.

Hitherto explored organic semiconductors often suffer from degradation processes and defects especially when electrochemically altered (“doped”), due to dopant drift and migration or due to oxidation when exposed to atmospheric conditions. The unique properties of poly(triazine imide) enable the research to address the issues that plague conventional organic semiconductors. Poly(triazine imide) is a very stable under heat and air. Furthermore, the graphitic morphology of poly(triazine imide) allows exfoliation of the material into thin, solution-processable layers, while at the same time reducing migration and drift of chemically bonded dopants. “With the improved material quality, we are now able to dive deeper into the more delicate features of this material, such as the electronic structure and vibration modes. This will greatly



improve our understanding of this material, as well as related materials, and help us improving OLED performance and think about future, high-value applications of poly(triazine imide).”, says David Burmeister, PhD student at IRIS Adlershof member Michael J. Bojdys.

**Optimized synthesis of solution-processable crystalline poly(triazine imide) with minimized defects for OLED application**

D. Burmeister, H.A. Tran, J. Müller, M. Guerrini, C. Cocchi, J. Plaickner, Z. Kochovski, E. List-Kratochvil, M. Bojdys  
*Angew. Chem. Int. Ed.*, 2021, 61(3), e202111749.  
DOI: 10.1002/anie.202111749

**PRINTING AN ELECTRONIC RAINBOW – COMBINATION OF COLOUR PRINTING AND CHEMICAL TUNABILITY ENABLES PRINTED SPECTROMETER**

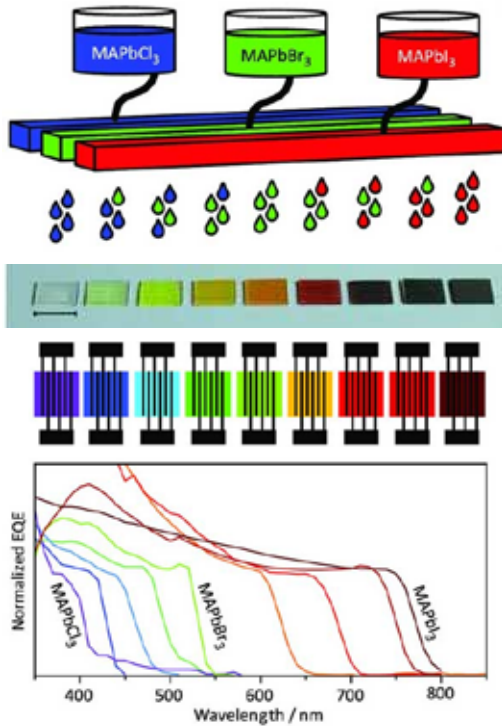
Researchers from Innovation Lab HySPRINT at Helmholtz-Zentrum Berlin (HZB) and Humboldt Universität zu Berlin (HU) have used an advanced inkjet printing technique to produce a large range of photodetector devices based on a hybrid perovskite semiconductor. By mixing of only three inks, the researchers were able to precisely tune the semiconductor properties during the printing process. Inkjet printing is already an established fabrication method in industry, allowing fast and cheap solution

processing. Extending the inkjet capabilities from large area coating towards combinatorial material synthesis opens the door for new possibilities for the fabrication of different kind of electronic components in a single printing step.

**Wonder material metal halide perovskites**

Metal halide perovskites are fascinating to researchers in academia and industry with the large range of possible applications. The fabrication of electronic components with this material





a) Combinatorial printing allows precise control of the mixing of perovskite precursor inks during film fabrication.

b) This leads to a compositional halide gradient in methylammonium-based metal halide perovskites.

c) Each perovskite composition is inkjet printed onto prefabricated interdigitated ITO electrodes to produce a series of nine photodetectors.

d) The detection onset of the photodetectors measured in external quantum efficiency directly relates to the compositional gradient of the metal halide perovskite.

is particularly appealing, because it is possible from solution, i.e. from an ink. Commercially available salts are dissolved in a solvent and then deposited on a substrate. The group around Prof. Emil List-Kratochvil, head of a joint research group at HZB and HU, focusses on building these types of devices using advanced fabrication methods such as inkjet printing. The printer spreads the ink on a substrate and, after drying, a thin semiconductor film forms. Combining multiple steps with different materials allows to produce solar cells, LEDs or photo-detectors in mere minutes.

Inkjet printing is already an established technique in industry, not only for newspapers and magazines, but also for functional materials. Metal halide perovskites are specifically interesting for inkjet printing, as their properties can be tuned by their chemical make-up. Researcher at HZB have already used inkjet

printing to fabricate solar cells and LEDs made from perovskites. The inkjet capabilities were further expanded in 2020, when the group of Eva Unger first used a combinatorial approach to inkjet printing, to print different perovskite compositions in search of a better solar cell material.

### **Combinatorial printing approach towards industrial production of electronic devices**

Now, in this current work, the team around Prof. Emil List-Kratochvil found an exciting application for a large perovskite series within wavelength-selective photodetector devices. “Combinatorial inkjet printing cannot only be used to screen different compositions of materials for solar cell materials,” he explains, “but also enables us to fabricate multiple, separate devices in a single printing step.” Looking towards an industrial process, this would enable large scale production of multiple electronic devices. Combined with printed electronic

circuits, the photodetectors would form a simple spectrometer: paper thin, printed on any surface, potentially flexible, without the need of a prism or grid to separate the incoming wavelengths.

### **Using Combinatorial Inkjet Printing for Synthesis and Deposition of Metal Halide Perovskites in Wavelength-Selective Photodetectors**

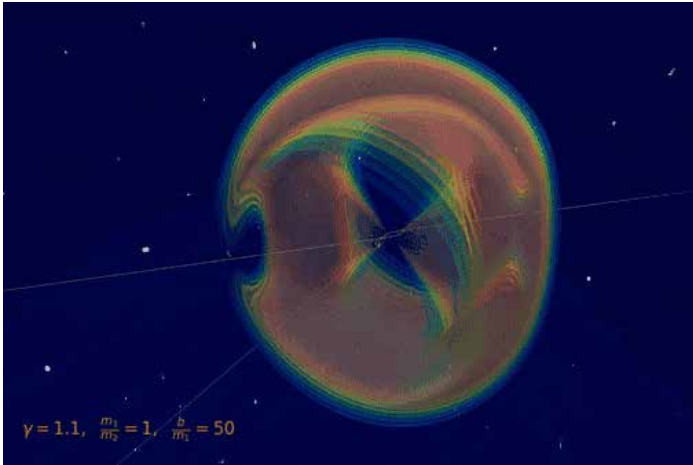
V.R.F. Schröder, F. Hermerschmidt, S. Helper, C. Rehermann, G. Ligorio, H. Näsström, E.L. Unger, and E.J.W. List-Kratochvil  
*Adv. Eng. Mater.*, 2021, 24(4), 2101111.  
DOI: 10.1002/adem.202101111

## **BREMSSTRAHLUNG OF BLACK HOLES AND NEUTRON STARS FROM QUANTUM FIELD THEORY**

When two massive objects (black holes, neutron stars or stars) fly past each other, the gravitational interactions not only deflect their orbits, but also produce gravitational radiation, or gravitational bremsstrahlung, analogous to electromagnetism. The resulting gravitational waves of such a scattering event were calculated at leading order in Newton's gravitational constant in the 1970s using traditional methods of

general relativity in an extensive series of four papers. Bremsstrahlung events are still out of reach for the current generation of gravitational-wave detectors because the signal is non-periodic and typically less intense. Nevertheless, they are interesting targets for future searches with future terrestrial and space-based observatories.

In the Quantum Field Theory lab around IRIS Adlerhof-member Prof. Plefka, a new



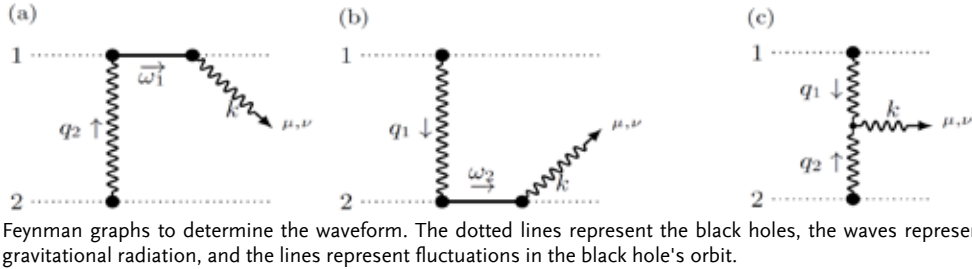
Visualization of the gravitational Bremsstrahlung from the scattering of two black holes (BSc thesis O. Babayemi)

approach to determining these waveforms and the deflections using methods of perturbative quantum field theory was recently developed, which proves to be significantly more efficient than the traditional approaches. It is based on a

hybrid quantum field theory, in which the black holes (or stars) are idealized as point particles and interact with the gravitational field. The calculation is then based on a systematic diagrammatic expansion using Feynman graphs. I.e. the methods that were originally developed for the scattering of elementary particles can now also be used in astrophysical scenarios.

With this innovative method - the "Worldline Quantum Field Theory" approach - our understanding of this fundamental physical process was recently significantly extended

resulting in a series of three publications in the Physical Review Letters. In [1], the results from the 1970s were reproduced in a far more efficient way; this only required the calculation of three Feynman graphs. In [2] the waveform could be



extended to the case of rotating black holes and neutron stars. In a recent publication [3], the scattering angles and deflections in momenta and rotations due to the scattering process at the next-next-leading order of the gravitational constant were determined for the first time. Elaborated techniques for calculating Feynman integrals were used here. Interestingly, the rotational degrees of freedom of the black holes are described in this new formulation with a supersymmetric world line theory [4], which was originally developed in extensions of the Standard Model of particle physics.

[1] **Classical Gravitational Bremsstrahlung from a Worldline Quantum Field Theory**

G. U. Jakobsen, G. Mogull, J. Plefka, and J. Steinhoff  
*Phys. Rev. Lett.*, 2021, 126(20), 201103.  
 arXiv: 2101.12688

[2] **Gravitational Bremsstrahlung and Hidden Supersymmetry of Spinning Bodies**

G. U. Jakobsen, G. Mogull, J. Plefka, and J. Steinhoff  
*Phys. Rev. Lett.*, 2022, 128(1), 011101.  
 arXiv: 2106.10256

**[3] Conservative and radiative dynamics of spinning bodies at third post-Minkowskian order using worldline quantum field theory**

G. U. Jakobsen and G. Mogull

*Phys. Rev. Lett.*, 2022, 128(14), 141102.

arXiv: 2201.07778

**[4] SUSY in the sky with gravitons**

G. U. Jakobsen, G. Mogull, J. Plefka, and J. Steinhoff

*J. High Energy Phys.*, 2022, 2022(1), 27.

arXiv: 2109.04465

## FAIR RESEARCH DATA IN MATERIALS SCIENCES

The FAIRmat consortium led by Humboldt-Universität zu Berlin describes its concept for accessible research data in the renowned journal Nature.

The lifestyle of our society is largely determined by the achievements of condensed matter physics, chemistry and material sciences. Touch screens, batteries, electronics or implants: Many new products in the fields of energy, environment, health, mobility and information technology are largely based on improved or even

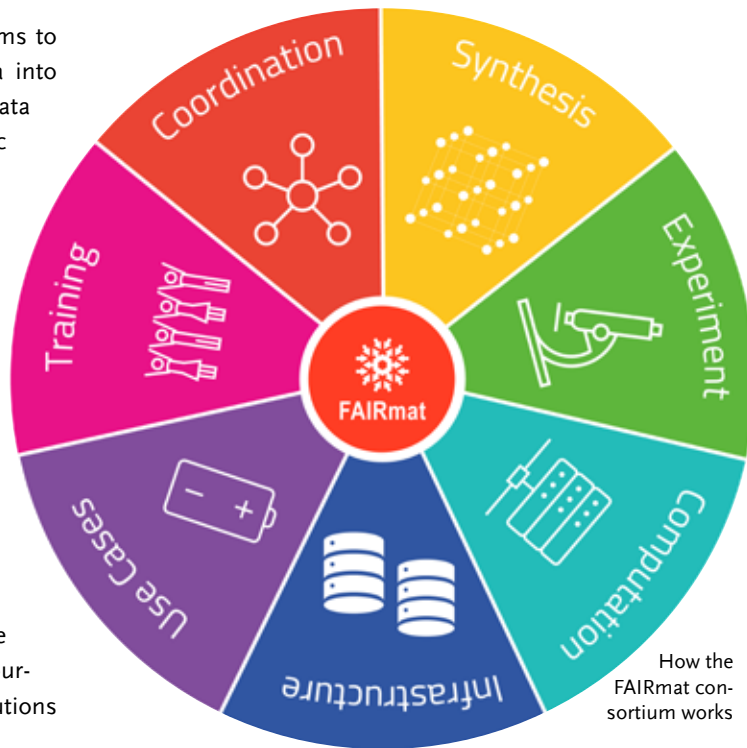
novel materials. These fields generate enormous amounts of data every day, which is a new raw material - and is therefore a gold mine in itself. However, a prerequisite for this is that these data are comprehensively characterized and made available to science.

### **FAIR data for shared use**

The FAIRmat consortium ("FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids"), led by IRIS

Adlershof member Prof. Claudia Draxl, aims to refine this raw material, i.e. turning data into knowledge and value. A prerequisite is a data infrastructure that makes enables scientific data to be „FAIR“, i.e. findable, accessible, interoperable and re-purposable. "With a "FAIR" infrastructure, data can be easily shared and explored using data analytics and artificial intelligence methods. This approach will significantly change the way how science is done today," says Claudia Draxl.

In the journal Nature, the scientists describe how such a data infrastructure can be successfully implemented in the field of materials science. The article appears today in the "Perspectives" format, in which the journal publishes forward-looking contributions



that stimulate discussion and new scientific approaches.

The FAIRmat consortium is part of the initiative “Nationale Forschungsdaten Infrastruktur” (NFDI). The project is based on the extensive experience with the world's largest data infrastructure in computational materials science, the Novel Materials Discovery (NOMAD) Laboratory, which was co-founded by Claudia Draxl and has been online since 2014. The main challenge for FAIRmat is the integration of many

different experimental characterization techniques and methods of material synthesis.

### **FAIR data enabling new horizons for materials research**

M. Scheffler, M. Aeschlimann, M. Albrecht, T. Bereau, H.-J. Bungartz, C. Felser, M. Greiner, A. Groß, C.T. Koch, K. Kremer, W.E. Nagel, M. Scheidgen, C. Wöll, and C. Draxl  
*Nature*, 2022, 604, 635.

DOI: 10.1038/s41586-022-04501-x

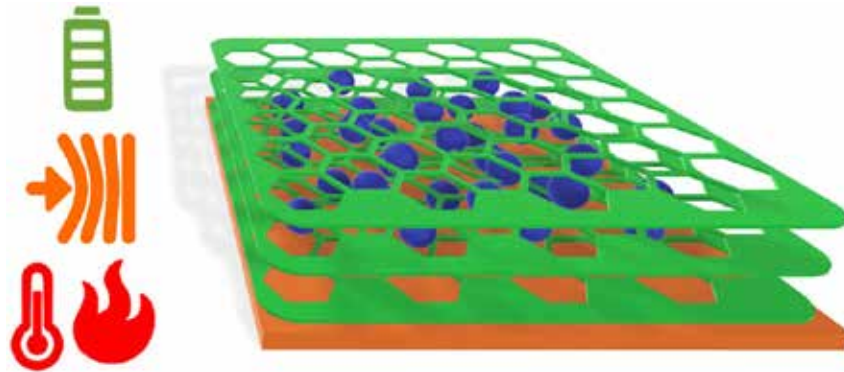


## NEW PRODUCTION METHOD FOR FLEXIBLE, DURABLE ANODES WITH HIGH CAPACITY-TO-WEIGHT

A team of researchers from Humboldt Universität zu Berlin, the Leibniz-Institut für Polymerforschung Dresden (IPF) e. V., and the Karlsruhe Institute of Technology (KIT) have made an anode with superior performance for portable battery applications,

close to limits of theoretical capacity. Uniquely, the obtained anodes are flexible without surface reconstruction or crack formation, and they survive heat shocks without performance-loss.

Conventional batteries break down when subjected to mechanical and thermal stress. As



a necessity, they need to be situated in stiff, rigid sections of nominally “foldable” electronics and away from sources of heat. The fundamental limitation of the conventional production methods is that the free motion of binders and additives used for battery assembly will lead, over time, to

a detrimental loss of the desired electrochemical bias, and finally to a dead battery. To overcome this limitation, the team of Prof. Michael J. Bojdys, the team leader at Humboldt Universität zu Berlin, had the idea to replace conventional binders and additives with a semi-conducting porous organic polymer that (i) adheres to the current collector and grows around the active material, and (ii) enables transport of electrolyte and charge-carriers.

Prof. Bojdys says “Batteries work because we carefully build a chemical bias from small particles. You see this represented in the plus-pole and minus-pole on the battery. Now, what happens if you start shaking or heating such an ordered system? Well, you destroy the chemical bias, and the battery is dead! The way how we build conventional batteries is comparable to putting all your shopping loosely into your car trunk – by the time you get home, everything is jumbled up. Now, if you want to keep

your shopping ordered, you obviously put it into bags! This is the role that our semi-conducting porous polymer plays in our electrodes. The polymer replaces all classic battery additives, and it leads to fantastic performance.”

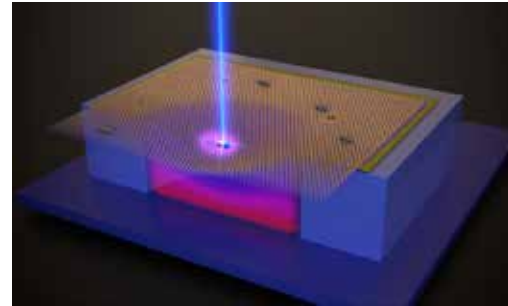
Based on this technology Dr. Goshtasp Cheraghian and Michael J. Bojdys seek to commercialize their electrodes and ink-formulations as part of the INAM AdMaLab 2022 Incubator Program.

### **One-pot synthesis of high-capacity silicon anodes via on-copper growth of a semiconducting, porous polymer**

J. Huang, A. Martin, A. Urbanski, R. Kulkarni, P. Amsalem, M. Exner, G. Li, J. Müller, D. Burmeister, N. Koch, T. Brezesinski, N. Pinna, P. Uhlmann, and M.J. Bojdys  
*Natural Sciences*, 2022, 2(3), e20210105.  
DOI: 10.1002/ntls.20210105

## ELECTRICALLY CONTROLLED STRAINING OF A SUSPENDED 2D SEMICONDUCTOR DRIVES DIFFERENT ENERGY STATES INTO HYBRIDIZATION, ENABLING SINGLE PHOTON EMISSION

Semiconducting, two-dimensional transition metal dichalcogenides (TMDs) have attracted much interest during the last 15 years. Their highly tuneable mechanical and optoelectronic properties and their combinability with other 2D materials into new structures make TMDs promising systems for many technologies such as electronics and power generation and storage. Their rich low dimensional physics include exotic phenomena as Bose-Einstein condensation or single photon emission, some of them not yet fully explained. Light-matter interaction in 2D semiconductors is governed by excitons, Coulomb-bound electron-hole pairs that can be classified as bright or dark depending on how strongly they couple with light. Despite being the ground state of the system, dark excitons in WSe<sub>2</sub> are now only starting to



be systematically studied. The group "Physics of Low Dimensional Systems" of Sebastian Heeg in HU Berlin in collaboration with AG Bolotin at FU Berlin and AG Libisch at TU Vienna have investigated the strain-dependence of dark excitons in monolayer WSe<sub>2</sub>. This system is particularly relevant as many studies have reported single photon emitters in strained WSe<sub>2</sub> but failed

to explain the microscopic mechanism underneath quantum light emission.

Sebastian Heeg explains how this project was originally conceived: “Our colleagues in the group of Florian Libisch from TU Vienna published in 2019 a very suggesting paper where they predicted that strain in single layer WSe<sub>2</sub> could bring dark excitons in resonance with naturally occurring defect energy levels. Once the two excitonic species were tuned into the same energy, they would combine their properties creating a hybridized state that enables single photon emission. When we read about this theoretical model, we immediately decided we wanted to probe it experimentally. To do so, we developed an electrostatic straining technique that allowed us to apply strain controllably at low and high temperatures on WSe<sub>2</sub> membranes while probing their electronic structure with photoluminescence spectroscopy.”

By applying strain on WSe<sub>2</sub> membranes with a high degree of control, the authors characterized the different excitonic species present in the material according to their energetic dependence with strain. At certain strain levels, strain-independent defect states and strain dependent dark excitons became energy degenerated and their photoluminescence intensity increased an order of magnitude. More evidence for the hybridization of the state such as avoided-crossing energy shifts and temperature tunability of the strain necessary to trigger hybridization was also reported. “The high tunability of the hybridized state enabled by our device architecture will be likely key for the operation of single quantum emitters in WSe<sub>2</sub>” highlights Pablo Hernández López, a doctoral candidate at Sebastian Dr. Heeg’s group and co-author of the paper, “On the other hand, the characterization and tuning of the energy hierarchy of the excitons present on suspended materials using our

electrostatic straining approach opens the door for more exciting discoveries in the future”.

**Strain control of hybridization between dark and localized excitons in a 2D semiconductor**

P. Hernández López, S. Heeg, C. Schattauer, S. Kovalchuk, A. Kumar, D.J. Bock, J.N. Kirchhof, B. Hofer, K. Greben, D. Yagodkin, L. Linhart, F. Libisch, K.I. Bolotin

Nature Communications, 2022, 13(1), 7691.

DOI: 10.1038/s41467-022-35352-9



## 3. Structure and Institutional Funding

### 3.1. IRIS Adlershof within the University Structure

Humboldt-Universität zu Berlin, 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. IRIS Adlershof is not part of a faculty.

#### INTEGRATIVE RESEARCH INSTITUTES – AN INNOVATIVE RESEARCH FORMAT

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 infrastructure 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.



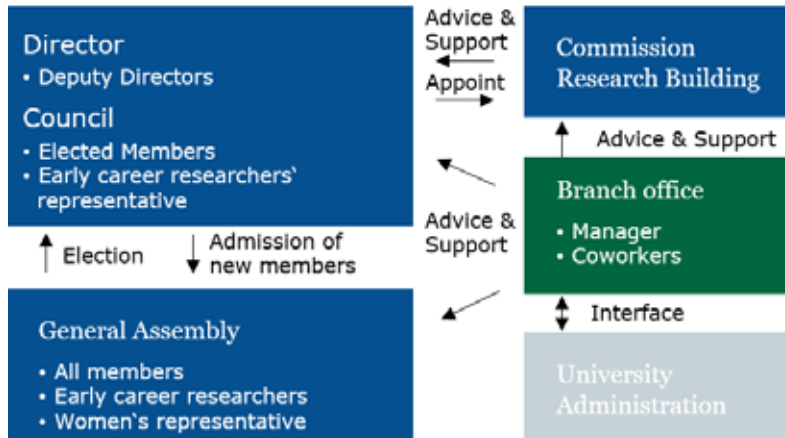
## ESTABLISHING COOPERATIONS WITH START UPS

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.

## 3.2. 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 scientific events 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.

#### ELECTED MEMBERS OF THE IRIS COUNCIL

As of end 2022, the IRIS Council consists of the following people:

- » Prof. Dr. Jürgen P. Rabe (Director)
- » Prof. Dr. Norbert Koch (Deputy Director)
- » Prof. Dr. Emil List-Kratochvil (Deputy Director)
- » Dr. Nikolai Puhlmann (Manager)
- » Prof. Dr. Claudia Draxl
- » Prof. Stefan Hecht, Ph.D.
- » Prof. Dr. Matthias Staudacher
- » Laura Orphal-Kobin  
(Representative of the Junior Researchers)

### 3.3. Members



Prof. Dr. Kannan Balasubramanian  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS-Member since 2017



Prof. Dr. Mathias Ballauff  
Freie Universität Berlin,  
Institute of Chemistry and Biochemistry  
IRIS-Member since 2010



Prof. Dr. Oliver Benson  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Founding Member (2008)



Prof. Dr. Michael J. Bojdys  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS Junior Member since 2018,  
IRIS-Member since 2021



Prof. Dr. Caterina Cocchi  
Carl von Ossietzky University of Oldenburg,  
Department of Physics and  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Member since 2017



Prof. Dr. Dr. h.c. Claudia Draxl  
Humboldt-Universität zu Berlin,  
Department of Physics and  
Fritz-Haber-Institut of the MPG  
IRIS-Member since 2012



Dr. Oliver Dumele  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS Junior Member since 2021,  
IRIS-Member since 2022



Prof. Dr. Thomas Elsässer  
Max Born Institute for  
Nonlinear Optics and Short Pulse  
Spectroscopy  
IRIS-Member since 2010



Valentina Forini, Ph.D.  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2018,  
IRIS Member since 2021



Prof. Dr. Michael Hintermüller  
Humboldt-Universität zu Berlin,  
Department of Mathematics and  
Weierstrass Institute (Weierstraß-Institut  
für angewandte Analysis und Stochastik)  
IRIS-Member since 2018



Dr. Nichol Furey  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2021,  
IRIS Member since 2022



Prof. Dr. Olaf Hohm  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Member since 2019



Prof. Stefan Hecht, Ph.D.  
Humboldt-Universität zu Berlin,  
Department of Chemistry and  
Leibniz Institute for Interactive Materials  
(DWI) and RWTH Aachen University  
IRIS-Founding Member (2008)



Prof. Christoph T. Koch, Ph.D.  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Member since 2016



Dr. Sebastian Heeg  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2021,  
IRIS-Member since 2022



Prof. Dr. Norbert Koch  
Humboldt-Universität zu Berlin,  
Department of Physics and  
Helmholtz-Zentrum Berlin für  
Materialien und Energie  
IRIS-Member since 2009



Prof. Dr. Jürg Kramer  
Humboldt-Universität zu Berlin,  
Department of Mathematics  
IRIS-Founding Member (2008)



Prof. Dr. Christian Limberg  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS-Member since 2014



Prof. Dr. Dirk Kreimer  
Humboldt-Universität zu Berlin,  
Department of Mathematics and  
Department of Physics  
IRIS-Member since 2011



Prof. Dr. Emil List-Kratochvil  
Humboldt-Universität zu Berlin,  
Department of Physics and  
Department of Chemistry  
IRIS-Member since 2015



Dr. Markus Krutzik  
Humboldt-Universität zu Berlin,  
Department of Physics and  
Ferdinand-Braun-Institut, Leibniz-Institut für  
Höchstfrequenztechnik  
IRIS Junior Member since 2021,  
IRIS-Member since 2022



Prof. Dr. Yan Lu  
Helmholtz-Zentrum Berlin für  
Materialien und Energie and  
University of Potsdam,  
Institute of Chemistry  
IRIS-Member since 2017



Prof. Dr. Ulf Leser  
Humboldt-Universität zu Berlin,  
Department of Computer Science  
IRIS-Member since 2021



Dr. Emanuel Malek  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2021  
IRIS-Member since 2022



Prof. Dr. Nicola Pinna  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS-Member since 2016



Prof. Dr. Matthias Scheffler  
Fritz-Haber-Institute (Max-Planck-  
Gesellschaft zur Förderung der  
Wissenschaften e.V.) and Humboldt-  
Universität zu Berlin, Department of Physics  
IRIS-Member since 2021



Prof. Dr. Jan Plefka  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Member since 2012



Dr. Tim Schröder  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS-Member since 2019



Prof. Dr. Jürgen P. Rabe  
Humboldt-Universität zu Berlin,  
Department of Physics and  
Max Planck Institute for  
Colloids and Interfaces  
IRIS-Founding Director



Prof. Dr. Igor M. Sokolov  
Humboldt-Universität zu Berlin,  
Department of Physics,  
IRIS-Member since 2017



Dr. Sven Ramelow  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2016  
IRIS-Member since 2022



Prof. Dr. Julia Stähler  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
IRIS-Member since 2021



Prof. Dr. Matthias Staudacher  
Humboldt-Universität zu Berlin,  
Department of Mathematics and  
Department of Physics  
IRIS-Member since 2010



Prof. Dr. Eva Unger  
Humboldt-Universität zu Berlin,  
Department of Chemistry  
Helmholtz-Zentrum Berlin für  
Materialien und Energie GmbH  
IRIS-Member since 2021



Dr. Stijn van Tongeren  
Humboldt-Universität zu Berlin,  
Department of Physics  
IRIS Junior Member since 2021  
IRIS-Member since 2022



## 3.4. Infrastructure of IRIS Adlershof

Finally, the grand opening of the IRIS Adlershof research building, jointly financed by the Federal Government, the State of Berlin and Humboldt-Universität zu Berlin, took place on October 5th, 2022 in the presence of Berlins Senator for Science, Health, Nursing and Equal Opportunities, Ms. Ulrike Gote, and the HU President, Prof. Julia von Blumenthal.

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. With the Research Building, IRIS Adlershof offers its

members excellent working conditions through its new laboratories and the provision of high-end, state-of-the-art 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 m<sup>2</sup> of laboratory space and 2,200 m<sup>2</sup> 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.

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 clean-room, a 19 m long glove-box 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 opening of the Research Building was a central milestone for IRIS Adlershof. The building promotes 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 Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) and the Fritz Haber Institute of the Max Planck Society (FHI), is based in the new building. As part of the AdMaLab program, lab spaces could be offered to collaborating startups like *C1 Green Chemicals AG* or *Theion*.

## 3.5. 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 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.

## 4. Research Areas

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 competence fields encourages close cooperation across the interdisciplinary boundaries of physics, chemistry, mathematics, and computer sciences.

IRIS Adlershof has particularly focused from its beginning in 2009 on two main areas:

*Hybrid Systems for Optics and Electronics, & Mathematical Physics of Space–Time–Matter.*

Since then, IRIS Adlershof expanded and the following three new research areas have been added:

*Big Data, Quantum technology, & Catalysis Research.*

### 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.

## 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 analyse 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 single coherent theory. Hopefully, it will become clear along the way how the smooth world that we experience emerges from the chaotic principles of quantum physics. Mathematicians and theoretical physicists are cooperating to address specific questions of mathematical physics in the described framework.

## BIG DATA

Big data is becoming increasingly important to material science because it enables researchers to analyse large amounts of complex data and extract valuable insights that can inform the development of new materials and technologies.

Materials science is a field that seeks to understand the properties and behaviour of different types of materials, and to use this knowledge to create new materials with desired properties. Big data can help in this process by providing access to vast amounts of data from a wide range of sources, such as experimental measurements, simulations, and literature.

On the other hand, a large database of material properties has to be provided and be designed as a FAIR (Findable, Accessible, Interoperable, and Re-purposable).

## QUANTUM TECHNOLOGY

Quantum technology is important because it has the potential to revolutionize the way we process, store, and transmit information. Unlike classical computing, which is based on binary bits, quantum computing is based on qubits, which can exist in multiple states at the same time. This allows quantum computers to perform certain tasks much faster than classical computers, such as factor large numbers and simulate complex systems.

In addition, quantum technology can also be used for secure communication, as quantum mechanics ensures that any attempt to intercept the information will be detected. Other potential applications of quantum technology include quantum cryptography, quantum sensors, and quantum materials.

The field has gained significant attention due to the Nobel Prize 2022.

## CATALYSIS RESEARCH

Catalysis research is important because it plays a critical role in advancing many key areas of modern science and technology. Catalysis is the process of accelerating a chemical reaction by introducing a catalyst, which lowers the activation energy required for the reaction to occur. This has a wide range of applications in fields such as energy, materials science, and environmental science.

For example, catalysis is used to convert with renewable resources, such as biomass and solar energy, water into hydrogen and build a climate-neutral economy. A hotspot for catalysis research has been developing in Berlin's research landscape for some time.





## 5. IRIS-Publications in High Impact Journals

### NATURE FAMILY

"Axial Localization and Tracking of Self-interference Nanoparticles by Lateral Point Spread Functions",

Y. Liu, Z. Zhou, F. Wang, G. Kewes, S. Wen, S. Burger, M. Ebrahimi Wakiani, P. Xi, J. Yang, X. Yang, O. Benson, and D. Jin,  
*Nature Communications*, 12 (2021) 2019.  
DOI: 10.1038/s41467-021-22283-0

"Direct observation of the particle exchange phase of photons",

K. Tschernig, C. Müller, M. Smoor, T. Kroh, J. Wolters, O. Benson, K. Busch, and A. Perez-Leija,  
*Nature Photonics*, 15 9 (2021) 671.  
DOI: 10.1038/s41566-021-00818-7

"Ultracold atom interferometry in space",  
M. D. Lachmann, H. Ahlers, D. Becker, A. N. Dinkelaker, J. Grosse, O. Hellmig, H. Müntinga, V. Schkolnik, S. T. Seidel, T. Wendrich, A. Wenzlawski, B. Carrick, N. Gaaloul, D. Lüdtke, C. Braxmaier, W. Ertmer, M. Krutzik, C. Lämmerzahl, A. Peters, W. P. Schleich, K. Sengstock, A. Wicht, P. Windpassinger, and E. M. Rasel,  
*Nature Communications*, 12 (2021) 1317.  
DOI: 10.1038/s41467-021-21628-z

"Band gap engineering in blended organic semiconductor films based on dielectric interactions",  
K. Ortstein, S. Hutsch, M. Hamsch, K. Tvingstedt, B. Wegner, J. Benduhn, J. Kublitski, M. Schwarze, S. Schellhammer, F. Talnack, A. Vogt,

P. Bäuerle, N. Koch, S. C. B. Mannsfeld, H. Kleemann, F. Ortmann, and K. Leo, *Nature Materials*, 20 (2021) 1407. DOI: 10.1038/s41563-021-01025-z

"An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles",

T. J. Jacobsson, A. Hultqvist, A. García-Fernández, A. Anand, A. Al-Ashouri, A. Hagfeldt, A. Crovetto, A. Abate, A. G. Ricciardulli, A. Vijayan, A. Kulkarni, A. Y. Anderson, B. P. Darwich, B. Yang, B. L. Coles, C. A. R. Perini, C. Rehermann, D. Ramirez, D. Fairen-Jimenez, D. Di Girolamo, D. Jia, E. Avila, E. J. Juarez-Perez, F. Baumann, F. Mathies, G. S. A. González, G. Boschloo, G. Nasti, G. Paramasivam, G. Martínez-Denegri, H. Näsström, H. Michaels, H. Köbler, H. Wu, I. Benesperi, M. I. Dar, I. B. Pehlivan, I. E. Gould, J. N. Vagott, J. Dagar, J. Kettle, J. Yang, J. Li, J. A. Smith, J. Pascual, J. J. Jerónimo-Rendón,

J. Felipe Montoya, J.-P. Correa-Baena, J. Qiu, J. Wang, K. Sveinbjörnsson, K. Hirslandt, K. Dey, K. Frohna, L. Mathies, L. A. Castriotta, M. H. Aldamasy, M. Vasquez-Montoya, M. A. Ruiz-Preciado, M. A. Flatken, M. V. Khenkin, M. Grischek, M. Kedia, M. I. Saliba, M. Anaya, M. Veldhoen, N. Arora, O. Shargaieva, O. Maus, O. S. Game, O. Yudilevich, P. Fassel, Q. Zhou, R. Betancur, R. Munir, R. Patidar, S. D. Stranks, S. Alam, S. Kar, T. Unold, T. Abzieher, T. Edvinsson, T. W. David, U. W. Paetzold, W. Zia, W. Fu, W. Zuo, V. R. F. Schröder, W. Tress, X. Zhang, Yu-Hsien Chiang, Z. Iqbal, Z. Xie, and E. Unger, *Nature Energy*, 7 (2022) 107. DOI: 10.1038/s41560-021-00941-3

"FAIR data enabling new horizons for materials research",

M. Scheffler, M. Aeschlimann, M. Albrecht, T. Berau, H. Bungartz, C. Felser, M. Greiner,

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*Nature*, 604 (2022) 635.  
DOI: 10.1038/s41586-022-04501-x

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C. Ozsoy-Keskinbora, W. Van den Broek,  
C. B. Boothroyd, R. E. Dunin-Borkowski, P. A. van  
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DOI: 10.1038/s41598-022-17373-y

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X. Zhang, F. Gaerisch, Z. Chen, Y. Hu, Z. Wang, Y.  
Wang, L. Xie, J. Chen, J. Li, J.V. Barth, A. Narita, E.  
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*Nature Communications*, 13 (2022) 442.  
DOI: 10.1038/s41467-021-27600-1

"A consistent picture of excitations in cubic  
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pervised learning from materials data",  
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C. Draxl,  
*Scientific Data*, 9 (2022) 646.  
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lithic perovskite–silicon tandem solar cells",  
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K. Jäger, D. Yoo, F. Lang, M. Grischek, B. Li, J. Li,  
O. Shargaieva, E. Unger, A. Al-Ashouri, E. Köhnen,

M. Stolterfoht, D. Neher, R. Schlatmann, B. Rech,  
B. Stannowski, S. Albrecht, and C. Becker,  
*Nature Nanotechnology*, 17 (2022) 1214.  
DOI: 10.1038/s41565-022-01228-8

"Vortex dynamics in the two-dimensional BCS-BEC  
crossover",  
M. Heyl, K. Adachi, Y. M. Itahashi, Y. Nakagawa,  
Y. Kasahara, E. J. W. List-Kratochvil, Y. Kato, and Y.  
Iwasa,  
*Nature Communications*, 13 (2022) 6986.  
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"Strain control of hybridization between dark and  
localized excitons in a 2D semiconductor",  
P. H. López, S. Heeg, C. Schattauer, S. Kovalchuk,  
A. Kumar, D. J. Bock, J. N. Kirchof, B. Höfer,  
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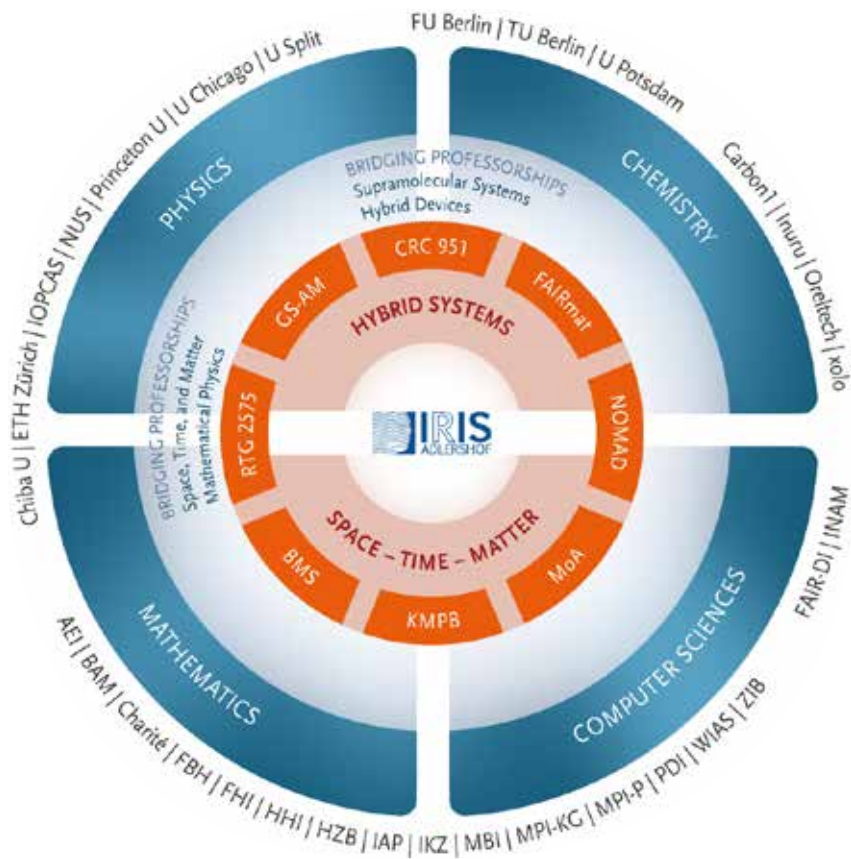
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## 6. Cooperation partners

|            |   |           |   |
|------------|---|-----------|---|
| AEI        | Max-Planck-Institut für Gravitationsphysik (Albert-Einstein-Institut)   | FHI       | Fritz-Haber-Institut der Max-Planck-Gesellschaft                    |
| BAM        | Bundesanstalt für Materialforschung und -prüfung  | FU Berlin | Freie Universität Berlin  |
| BMS        | Berlin Mathematical School  | GS-AM     | Graduate School "Advanced Materials"                                |
| Carbon1    | C1 Green Chemicals AG   | HHI       | Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut |
| Charité    | Charité – Universitätsmedizin Berlin  | HZB       | Helmholtz-Zentrum Berlin für Materialien und Energie GmbH           |
| Chiba U    | Chiba University - Graduate School of Advanced Integration Science  | IAP       | Fraunhofer-Institut für Angewandte Polymerforschung                 |
| CRC 951    | Collaborative Research Center (Sonderforschungsbereich) 951 Hybrid Inorganic/Organic Systems for Opto-Electronics | IKZ       | Leibniz Institut für Kristallzüchtung                               |
| ETH Zürich | Eidgenössische Technische Hochschule Zürich   | INAM      | Innovation Network for Advanced Materials                           |
| FAIRmat    | FAIRmat   | IOPCAS    | Institute of Physics, Chinese Academy of Sciences                   |
| FBH        | Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik  | KMPB      | Kolleg Mathematik und Physik Berlin                                 |
|            |   | MoA       | Exzellenzcluster "Matters of Activity, Image Space Material"        |

|           |  |
|-----------|--|
| MBI       | Max-Born-Institut für Nichtlineare Optik<br>und Kurzeitspektroskopie |
| MPI-KG    | Max-Planck-Institut für Kolloid- und Grenz-<br>flächenforschung      |
| MPI-P     | Max-Planck-Institut für Polymerforschung                             |
| NOMAD     | Novel Materials Discovery  |
| NUS       | National University of Singapore                                     |
| OrelTech  | OrelTech GmbH  |
| PDI       | Paul-Drude-Institut für Festkörperelektronik                         |
| Princeton | Princeton University   |
| RTG 2575  | Research Training Group 2575 - Rethinking<br>Quantum Field Theory    |
| TU Berlin | Technische Universität Berlin  |
| U Chicago | University of Chicago  |
| U Potsdam | Universität Potsdam  |
| U Split   | University of Split  |
| WIAS      | WIAS - Weierstraß-Institut für Angewandte<br>Analysis und Stochastik |
| xolo      | xolo GmbH  |
| ZIB       | Konrad-Zuse-Zentrum für Informationstech-<br>nik Berlin              |

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