IRIS ADLERSHOF

IRIS Adlershof

2009 – 2024

Preface

Since its founding in 2009, the *Integrative Research Institute for the Sciences* at Humboldt-Universität zu Berlin – IRIS Adlershof – can now look back on 15 years of successful work.

During this time, IRIS Adlershof has grown into an internationally recognized and widely visible player in the fields of *Hybrid Systems for Optics and Electronics*, as well as in *Mathematical Physics of Space-Time-Matter*. In addition, new research areas such as *Big Data*, *Quantum Technology*, and *Catalysis Research* have been established and networked.

From its inception, IRIS Adlershof was conceived as an innovative yet temporary university structure that would connect existing core competencies of university research with non-university partners in research and industry, create a powerful framework for forward-looking interdisciplinary collaborative projects, and promote the development of young scientists. We see ourselves as a driving force for innovation, interdisciplinary cooperation in scientific research, application, and training of the next generation of scientists.

International review committees have confirmed that we have more than lived up to this expectation. This makes us a little proud and gives us optimism for the future, even as IRIS Adlershof will come to an end on October 31, 2024.

With the acquisition, construction, and commissioning of the highly innovative IRIS research building, as well as the establishment of the *Kolleg Mathematik Physik Berlin (KMPB)* and the *Center for the Science of Materials Berlin (CSMB)*, we have laid important preconditions for the continued successful development of interdisciplinary scientific research at the Adlershof campus of Humboldt-Universität zu Berlin.

The idea of IRIS Adlershof will therefore continue to live on in the future.

It is our great 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.

Sincerely,

Jürgen P. Rabe & Nikolai Puhlmann

Content

I. Executive Summary

The key milestones, scientific achievements, and strategic developments of IRIS Adlershof from its foundation in 2009 to today's Finissage (October 2024) are highlighted, providing a comprehensive overview of over a decade of pioneering research, infrastructural growth, and international collaboration.

Starting in 2009, Humboldt-Universität (HU) has established Integrative Research Institutes (IRI) as part of its Institutional Strategy, which was later funded by the federal and state governments as part of the second round of the Excellence Initiative. They were intended to facilitate and promote cutting-edge research by building bridges between different disciplines. An important aim of these innovative structures was to link HU's existing core competencies with external research and industry partners in order to create an efficient structure for promising interdisciplinary cooperation projects and to promote the development of young scientists. The HU has thus also responded to the so-called "pillarization" of the German higher education and science system, which still makes it difficult to optimally exploit the existing research potential at the interface between university and non-university research institutions.

The first IRI, the *Integrative Research Institute for the Sciences IRIS Adlershof*, was established on HU's natural science campus at Berlin-Brandenburg's top science, business, and media hub Berlin-Adlershof in Summer 2009. IRIS brought together the core competences of modern optics, molecular systems, mathematical physics, and computation in the sciences. The integrative nature of IRIS Adlershof was additionally strengthened by specifically hiring professors to bridge between the established disciplines, physics, chemistry, and mathematics.

IRIS Adlershof combines elements of a research institute, a development laboratory, and an institute for advanced studies and sustainably links Humboldt-Universität with pertinent non-university institutions and innovative enterprises. It has focused from its beginning on two main areas of research: *Hybrid Systems for Optics and Electronics* and *Mathematical Physics of Space–Time–Matter*. In the course of its further development, the spectrum of IRIS Adlershof has been expanded to include the research fields of *Big Data*, *Quantum Technology*, and *Catalysis Research*. In addition, IRIS Adlershof has devoted itself to new, cross-disciplinary perspectives with the *Cluster of Excellence EXC 1027 Image Knowledge Gestaltung* and its successor *EXC 2025 Matters of Activity. Image–Space–Material*, which go beyond the two research areas *Hybrid Systems for Optics and Electronics* and *Mathematical Physics of Space–Time–Matter*, and at the same time link them.

Initially housed in one small office at the department of physics, the new institute faced challenges in securing adequate space for its research endeavours. In 2010, the state of Berlin transferred a former barracks site to Humboldt-Universität, providing a permanent home for IRIS Adlershof, creating space for theoretical research and collaborative initiatives. To address the increasing demand for experimental research space, IRIS initiated the successful application of the State of Berlin for a research building dedicated to hybrid systems in electronics and photonics, which was completed in 2020.

IRIS Adlershof underwent two successful evaluations by international expert panels, which highlighted the success in the institute's achievements and commitment to internationalization, research excellence, and strategic development. These evaluations secured extensions of IRIS' basic funding and operations until 2024. The consistent flow of over 100 million euros in third-party further fuelled the institute's growth and ensured the continuation of cutting-edge research.

Throughout its years of operation, IRIS Adlershof consistently produced high-quality research, with members publishing over 180 peer-reviewed articles annually in prestigious journals. Ground breaking work, such as advancements in doping in organic semiconductors or molecular switching in hybrid superlattices, further established the institute as a leader in its field.

IRIS Adlershof's international reputation grew as it fostered collaborations with leading research institutions worldwide. Partnerships with prestigious international universities such as *Princeton University*, the *National University of Singapore*, *Tel Aviv University*, the *Pritzker School of Molecular Engineering* strengthened its global network considerably. IRIS also welcomed numerous distinguished guest researchers, further enhancing its visibility and research output. Particularly noteworthy is the cooperation between IRIS Adlershof and the *Institute of Physics of the Chinese Academy of Sciences*. The most visible result of this international cooperation 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.

The promotion of young scientists has been an important focus of IRIS Adlershof's work from the very beginning. For example, all IRIS Members taught in the study programs of their departments and also gave special lectures in order to better communicate the research of IRIS Adlershof. Furthermore, IRIS Adlershof increased its commitment to the existing master programs *Polymer Science* and *Optical Science*. The promotion of early-career researchers at IRIS Adlershof was enhanced by the implementation of new doctoral programs in the IRIS research areas – the *Graduate School Advanced Materials* in the research area *Hybrid Systems for Optics and Electronics* and the *RTG 2575 Rethinking*

Quantum Field Theory in the research area *Mathematical Physics of Space–Time–Matter*. Both programs have been in operation since spring 2020 and offer early-career researchers excellent career-building opportunities, both in scientific and transferable skills. EU training programs, such as *Scattering Amplitudes: from Geometry to EXperiment SAGEX*, in which IRIS Adlershof was involved through its members, provided additional strong components for the promotion of early-career. IRIS also offered administrative and financial support to its early-career researchers. As a service provider in science management, IRIS Adlershof assisted them, for example, in setting up their working groups or in organizing scientific events. Within the institutional scope of available funds, IRIS Adlershof awarded fellowships to early-career researchers and issued a corresponding guideline in May 2020. The fellowship was intended to allow recipients to dedicate themselves fully to completing their research projects or applying for third-party funds. Many of these measures were the result of direct suggestions from our early-career researchers, who were involved in the IRIS committees via elected representatives and thus had a seat and vote on the IRIS Council and in the General Assembly. This ensured that the interests and concerns of early-career researchers were taken into account, when decisions were made.

Beyond academic research, IRIS Adlershof has played a pivotal role in promoting Berlin as a center for innovation and start-ups. Through its partnerships with the *Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB)* and as a co-founder of the *Innovation Network for Advanced Materials*

(INAM), the institute supported incubator programs such as AdMaLab, fostering the translation of scientific discoveries into real-world applications. Successful start-ups with a strong connection are for example *C1 Green Chemicals AG*, *Inuru GmbH* and *xolo GmbH*.

IRIS Adlershof sees itself as a place of diversity, plurality of opinion, mutual appreciation, and respect. Therefore, IRIS Adlershof has always attached great importance to the provision of equal opportunities. Since female scientists are unfortunately still underrepresented in some disciplines of natural sciences, including physics, IRIS Adlershof provided particular administrative and financial support to its female scientists. Promising female doctoral students were actively supported in taking the next step in their academic careers by receiving interim funding and scholarships that enabled them to start and successfully complete a doctorate and publish their results in international journals. Three female IRIS junior research group leaders – Caterina Cocchi, Valentina Forini, Yan Lu – accepted calls for permanent academic positions as university professors.

While IRIS Adlershof is concluding, its legacy will remain through its extensive publications, the ongoing projects *Kolleg Mathematik Physik Berlin* (KMPB) and *Center for the Science of Materials Berlin* (CSMB), its enduring research building, and the global network of scientists, it has inspired.

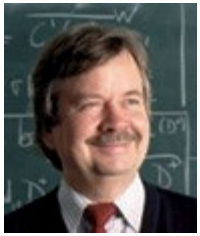
2. People

This chronological list of IRIS Adlershof members beautifully illustrates the institute's development over the past 15 years.

Founded in July 2009, IRIS Adlershof emerged from the initiative of nine pioneering researchers from the fields of physics, mathematics, chemistry and computer science:

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

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



Brüning, Jochen, Prof. Dr.
Humboldt-Universität zu Berlin,
Department of Mathematics
IRIS-Founding Member, Member until 2021

Freytag, Johann-Christoph, Prof. Ph.D.
Humboldt-Universität zu Berlin,
Department of Computer Science
IRIS-Founding Member, Member until 2017

Hecht, Stefan, Prof. Ph.D.
Humboldt-Universität zu Berlin, Department of Chemistry
since 2019 until 2022 DWI - Leibniz Institute for Interactive Materials
& RWTH Aachen, Department of Chemistry, IRIS-Founding Member

Henneberger, Fritz, Prof. Dr. († 2015)
Humboldt-Universität zu Berlin,
Department of Physics
IRIS-Founding Member

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

Reinefeld, Alexander, Prof. Dr.
Zuse Institute Berlin (ZIB) and
Humboldt-Universität zu Berlin, Department of Computer Science
IRIS-Founding Member, Member until 2021

Sauer, Joachim, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Chemistry and
Fritz Haber Institute of the Max Planck Society
IRIS-Founding Member, Member until 2017

In the following years, the new integrative institute succeeded in attracting several important scientists. Particularly noteworthy is the involvement of scientific leaders from non-university research institutions, such as Thomas Elsässer, Director at the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, and Matthias Ballauff, Director at the Institute for Soft Matter and Functional Materials at the Helmholtz-Zentrum Berlin (HZB), as well as Norbert Koch, who heads a research group at the HZB in addition to his professorship at the HU.

Koch, Norbert, Prof. Dr. (Deputy Director since 2017)
Humboldt-Universität zu Berlin, Department of Physics and
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
IRIS Member since 2009

Ballauff, Matthias, Prof. Dr.
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH and
Freie Universität Berlin, Department of Chemistry und Biochemistry
IRIS Member since 2010

Elsässer, Thomas, Prof. Dr.
Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy and
Humboldt-Universität zu Berlin, Department of Physics
IRIS Member since 2010

Matthias Staudacher and Dirk Kreimer, the next two members, are notable for being the first professors appointed through joint appointment procedures between two departments at HU (Mathematics and Physics). Additionally, Emil List-Kratochvil, appointed in 2015, holds a third bridging professorship (Chemistry and Physics). This highlights IRIS Adlershof's strategy of focusing on expertise in the overlapping areas of Mathematics/Physics and Chemistry/Physics.

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

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

Draxl, Claudia, Prof. Dr. Dr. h.c.
Humboldt-Universität zu Berlin,
Department of Physics
IRIS Member since 2012

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

von Klitzing, Regine, Prof. Dr.
Technische Universität Berlin, Department of Chemistry
Since 2017 Technical University of Darmstadt, Department of Physics
IRIS Member since 2012 until 2017

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

List-Kratochvil, Emil, Prof. Dr. (Deputy Director since 2020)
Humboldt-Universität zu Berlin, Departments of Physics and of Chemistry
and Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
IRIS Member since 2015

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

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

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

Cocchi, Caterina, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Physics
since 2020 Carl von Ossietzky Universität Oldenburg, Department of Physics
IRIS Member since 2017

Lu, Yan, Prof. Dr.
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH and
Universität Potsdam, Department of Chemistry
since 2023 Friedrich Schiller University Jena
IRIS Member since 2017

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

In addition to welcoming more established scientists as full members, IRIS Adlershof has taken significant steps to support and integrate young researchers. In 2018, the institute launched the IRIS Junior Membership, an initiative designed to recognize and promote outstanding early-career scientists. The first recipients of this distinction were Michael Bojdys, Valentina Forini, and Sven Ramelow, each recognized for their exceptional contributions to their fields.

Bojdys, Michael J., Prof. Dr.
Humboldt-Universität zu Berlin, Department of Chemistry
from 2020 until 2023 King's College London
IRIS Junior Member since 2018, IRIS Member since 2021

Forini, Valentina, Prof. PhD
Humboldt-Universität zu Berlin, Department of Physics
from 2018 until 2023 City University London,
since 2023 professorship at HU's Physics department
IRIS Junior Member since 2018, IRIS Member since 2021

Ramelow, Sven, Dr.
Humboldt-Universität zu Berlin,
Department of Physics
IRIS Junior Member since 2018, IRIS Member since 2022

Hintermüller, Michael, Prof. Dr.
Weierstraß-Institute for Applied Analysis and Stochastics and
Humboldt-Universität zu Berlin, Department of Mathematics
IRIS Member since 2018

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

Schröder, Tim, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Physics and
Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik
IRIS Member since 2019

In preparation for the final funding period, several promising early-career scientists were offered junior memberships. Following the review committee's recommendation, the distinction between full and junior members, as originally outlined in the IRIS statutes, was abolished at the end of 2022. This change aimed to enhance the visibility of our junior members and acknowledge their crucial role in the scientific life of IRIS Adlershof. Consequently, all former junior members were promoted to full members, with the same rights and responsibilities.

Dumele, Oliver, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Chemistry
Since 2023 University of Freiburg, Institute of Organic Chemistry
IRIS Junior Member since 2021, IRIS Member since 2022

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

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

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

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

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

Scheffler, Matthias, Prof. Dr.
Fritz Haber Institute of the Max Planck Society and
Humboldt-Universität zu Berlin, Department of Physics
IRIS Member since 2021

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

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

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

Young Scientist Representatives

In 2017, a significant step was taken to enhance the visibility of young researchers through the establishment of a dedicated young scientists' role within the internal structure. These representatives, elected by the doctoral candidates and postdocs of the IRIS groups, serve as their voice in the General Assembly and the IRIS Council. They possess the rights to speak, propose initiatives, and vote, ensuring that the perspectives of early-career researchers are heard and valued. Additionally, they organized several events for their junior colleagues.

2017-2022:


The first young scientiststst representatives:
Julian Miczajka, doctoral student in the group of Jan Plefka, and his deputy, Sven Ramelow, Emmy-Noether Research Group Leader

2022-2024:

Laura Orphal-Kobin and her deputy, Pablo Hernández López facilitated social and scientific events with support from the IRIS Office. These initiatives were crucial for incorporating young scientists into the newly opened research building, particularly in the context of post-COVID restrictions.

The administrative office

Dr. Nikolai Puhlmann was involved in the founding and development of IRIS Adlershof from the very beginning. Over time, he succeeded in establishing an efficient and effective administrative office that supports the scientific members of IRIS.

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 they 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 such as the international conference Fπ14, and in managing the promotion of early-career researchers. This allows researchers at IRIS Adlershof to focus on their core tasks: scientific research and teaching.

3. 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.

When founded in 2009, IRIS Adlershof focused particularly on the following two main research areas: *Hybrid Systems for Optics and Electronics* and *Mathematical Physics of Space–Time–Matter*.

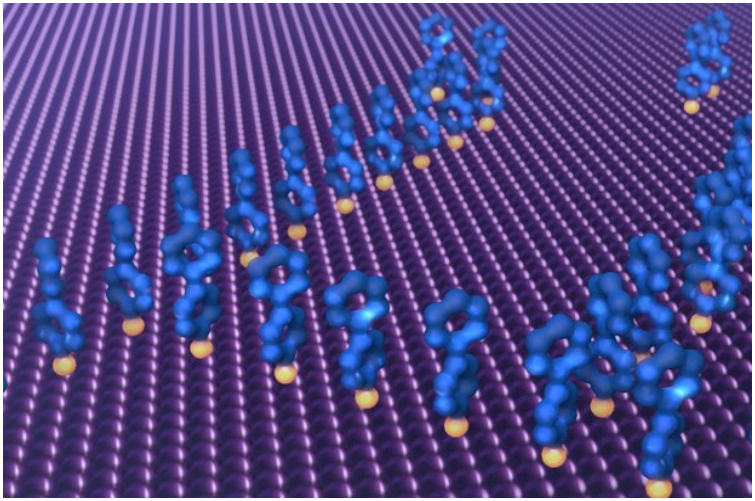
For the final funding period, IRIS Adlershof expanded into new research fields. This shift addressed recent scientific advancements and integrated emerging competencies at the campus and among IRIS Members. Building on the success of its interdisciplinary approach, bridging various fields, individuals, and institutions, IRIS Adlershof extended its strategy to include the following three areas:

Big Data, *Quantum Technology*, and *Catalysis Research*.

3.1. Hybrid Systems for Optics and Electronics

Hybrid inorganic/organic systems structured on atomic, molecular, and mesoscopic length scales provide 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.



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

The CRC 951: *Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS)* was the ıthouse project of IRIS Adlershof in this research area. The involvement of RIS Adlershof in the CRC was significant: HIOS was consistently headed by two IRIS Members as spokespersons, in the first funding period by the duo Fritz Henneberger / Norbert Koch, followed by Norbert Koch / Oliver Benson in the second and third period, respectively. A total of 13 IRIS Members were involved as PIs throughout the CRC's duration from 2011 to 2023.

Other key projects include the *Joint Laboratory for Structural Research*, which develops and provides infrastructure for studying organic, inorganic, and hybrid materials using advanced techniques such as microscopy, scattering, and lithography with electrons, X-rays, and scanning probes. The *HUMBOLDT ACCESS - Open Laboratory for Advanced Materials*, a platform designed to foster collaboration between IRIS Adlershof and relevant scientific and industrial partners, aimed to develop and implement tailored concepts for organic and molecular electronics. In addition, the working conditions for doctoral students in this research field have been significantly improved by the introduction of the *Graduate School Advanced Materials*.

In 2022, Humboldt-Universität zu Berlin founded the *Center for the Science of Materials Berlin (CSMB)* to further develop its strong expertise in this research field.

3.2. Mathematical Physics of Space–Time–Matter

Modern physics strives to understand from first principles the structure of space, time, and matter on very large and very small scales, as well as in complex systems. An important and challenging objective is to analyze the role of basic symmetries as well as the way they are broken. The ultimate goal is to discover the "Weltformel", a unified theory that describes fundamental forces and their interactions in a single framework. Mathematicians and theoretical physicists are cooperating to address specific questions of mathematical physics in the described framework.

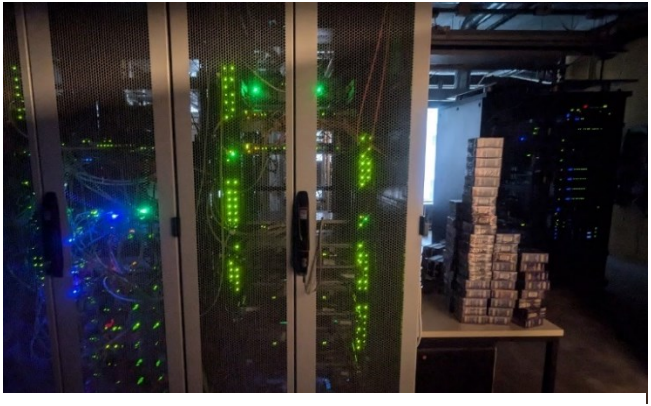
The lighthouse project within this research field was the *CRC 647: Space - Time - Matter: Analytic and Geometric Structures* (2005 - 2016), headed by the IRIS Members Jochen Brüning and Matthias Staudacher. It focused on creating a synthesis between mathematical and physical problem-solving. One of its key contributions was solving long-standing problems in general relativity, such as the classification of Lorentzian manifolds and the behavior of spacetime near singularities. Despite significant advances in unifying gravity and gauge theories, the ultimate goal of developing a unified "Theory of Everything", the so-called "Weltformel" remains an open and exciting challenge for the future.

Further important projects include the PhD program *International Max Planck Research School (IMPRS) for Mathematical and Physical Aspects of Gravitation, Cosmology and Quantum Field Theory*, the Marie Skłodowska-Curie Innovative Training Network *SAGEX - Scattering Amplitudes: from Geometry to Experiment*, and the DFG Research Training Group 2575 *Rethinking Quantum Field Theory*, that was extended in May 2024 by another four years. The strength in this research field culluminated in the founding of the Interdisciplinary Center *Kolleg Mathematik Physik Berlin (KMPB)*.

3.3. Big Data

IRIS Adlershof established a new research field in *Big Data*, intersecting physics, mathematics, computer science, chemistry, and materials science. IRIS Member Claudia Draxl has been a key figure in this effort, focusing on innovative big data management in computer-aided materials science from the beginning. She actively contributes to three major *Big Data* projects at the Adlershof campus: *NOMAD Lab*, *CRC 1404 FONDA*, and *FAIRmat*.

In close cooperation with IRIS Member Matthias Scheffler she has built up the Novel Materials Discovery Laboratory (*NOMAD Lab*), the world's largest database of material properties, which now contains more than 120 million calculations. Designed as a FAIR (Findable, Accessible, Interoperable, and Re-purposable) infrastructure, the NOMAD Lab enables the productive handling of scientific data and is thus, together with the use of Artificial Intelligence, essential for the



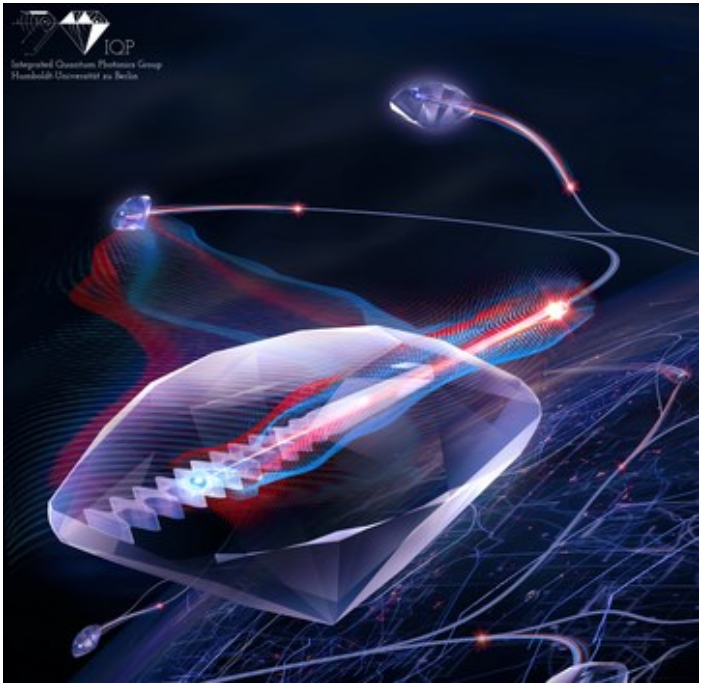
Computing Cluster in the Department of Physics

development of future technologies. As part of the NOMAD Center of Excellence, which was renewed for a second funding period in 2020, Draxl and Scheffler are also developing computational materials science into new applications and preparing it for the next generation of high-performance computers (exascale computers).

The next major project, led by IRIS Member Claudia Draxl, *FAIRmat*, is funded as a consortium of the *National Research Data Infrastructure (NFDI)*. It aims to develop and maintain a federated FAIR (Findable, Accessible, Interoperable, and Re-usable) data infrastructure for materials data with built-in tools and standards to support scientific collaboration and proper research data management practices. This initiative will enable researchers in Germany and around the world to store, share, find, and analyze data over the long term.

The *CRC 1404 FONDA – Foundations of Workflows for Large-Scale Scientific Data Analysis*, approved by the German Research Foundation in July 2020, advances IRIS Adlershof towards Big Data. An interdisciplinary team from computer science, material science, geosciences, and life sciences aims to boost productivity in developing, executing, and maintaining Data Analysis Workflows for large datasets. Spokesperson of the CRC is IRIS Member Ulf Leser from HU's Computer Science Department, with additional participation from IRIS Members Claudia Draxl and Christoph Koch.

3.4. Quantum Technology



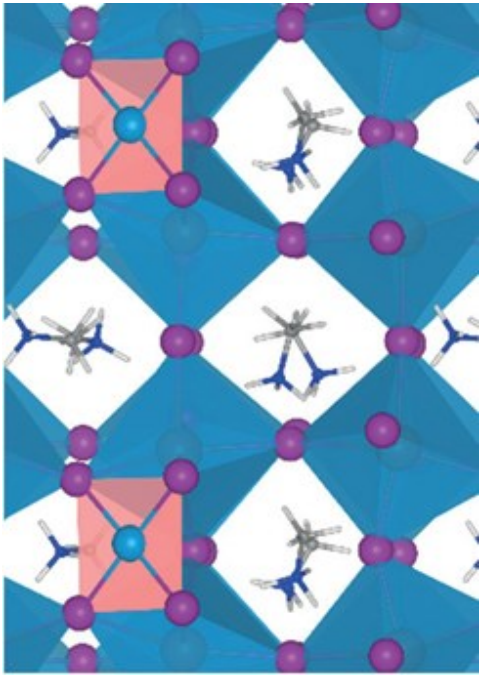
IRIS Adlershof expanded its spectrum towards a new field of research in Quantum Technology. The foundation for this was laid through Oliver Benson and Sven Ramelow, who described the first infrared based microscope with quantum light in a highly recognized article in Science Advances (DOI: 10.1126/sciadv.abd0264).

In 2018, this undertaking was further advanced by the granting and participation of Benson's and Ramelow's groups in the joint project *Quantum Link Expansion* (*Q.Link.X*) that has being funded by

the Federal Ministry of Education and Research. In *Q.Link.X* researchers explored the key technology of quantum repeaters. It was followed in 2021 by the BMBF joint research project *Quantenrepeater.Link* (*QR.X*) Two promising scientists of these projects became IRIS Members, Tim Schröder in 2019 and Markus Krutzik in 2021, also participate in these projects.

Quantum computers are seen as one of the key technologies of the 21st century. Can they revolutionize the computational capacity of computers? Which new insights do they offer for high energy physics or quantum chemistry? An interdisciplinary research team of the Berlin University Alliance partners, which includes IRIS Adlershof members Michael Hintermüller, Oliver Benson and Tim Schröder, has made it its task to explore the potential of the quantum digital transformation. As part of the first Einstein Research Group *Perspectives on digital quantum change: Near-term quantum computational devices and quantum processors* funded by the Einstein Foundation Berlin from 2021 to 2024, they combine expertise in theoretical and experimental physics, applied mathematics, computer science and machine learning in a unique way.

3.5. Catalysis Research



Catalysts are the key to many technologies and processes needed to build a climate-neutral economy. A hotspot for catalysis research has been developing in Berlin's research landscape for some time.

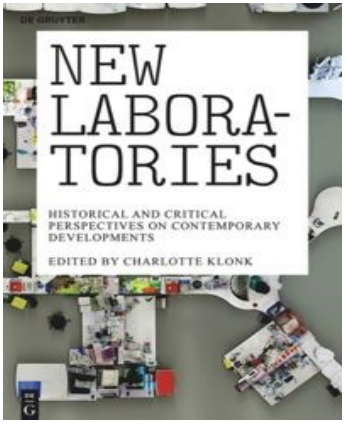
As part of the Excellence Strategy, new clusters such as *UniSysCat* have been created in which established research institutes bundle their activities and the chemical industry is involved through the *BASCat laboratory*. An important field of research is the production of green hydrogen: in order to produce hydrogen and synthetic fuels in a climate-neutral way using renewable energies, innovative catalysts are needed. The Berlin-based *CatLab* project, which is funded as part of the federal *Hydrogen Strategy*, is pursuing completely new approaches based on thin-film technologies that promise real leaps in innovation.

In order to make our energy system CO_2-neutral, the production of green hydrogen and its further processing into basic chemicals and synthetic fuels on an industrial global scale is absolutely necessary. However, such a hydrogen economy can only be achieved with innovative leaps in synthetic chemistry. Novel catalysts and catalytic processes are the key.

To further promote catalysis research in Berlin, HU, HZB and the Fritz Haber Institute of the Max Planck Society have agreed on close scientific cooperation. Some of the laboratories in the new IRIS research building were additionally equipped for the development and investigation of heterogeneous catalyst systems. To study catalysts in action, electron microscopes have been set up in the basement. In addition, in-operando investigation methods such as X-ray diffraction, photoelectron, Raman, and UV-vis spectroscopy were used, which could be completed by the high-end analysis options of the neighboring synchrotron radiation source BESSY II of the HZB. Close cooperation was also established in the field of thin-film technology, using additive manufacturing processes, nanostructuring, and synthesis methods.

Several startups have been working in the labs of IRIS Adlershof on catalysis, f.e. *C1 Green Chemicals*, founded in 2022, which is now building the world's first industrial-grade pilot-plant for cost-efficient green methanol production.

4. The IRIS Research Building



Planning a New Laboratory:
The Integrative Research Institute for the Sciences IRIS in Berlin

Jürgen P. Rabe

in: New Laboratories - Historical and Critical Perspectives on Contemporary Developments

From the very beginning, IRIS aimed to create dedicated research spaces for its experimentally focused groups, which required not only office and meeting areas but also state-of-the-art laboratories. The research project *Gestaltung von Laboren* in the Cluster of Excellence *Image Knowledge Gestaltung. An Interdisciplinary Laboratory* commenced in parallel, and its findings significantly shaped the vision and structure of the research building. In June 2013, the Joint Science Council of the federal and state governments approved IRIS Adlershof's application for a new research building dedicated to *Hybrid Systems for Electronics, Optoelectronics, and Photonics*.

The successful completion and the gradual commissioning of the IRIS research building in early 2021 marked a significant milestone in the development of IRIS Adlershof, which has led to a noticeable improvement in its laboratory facilities and scientific infrastructure. Previously, the infrastructure did not allow for highly specialized laboratories to be set up in the existing IRIS building

at *Zum Großen Windkanal 6*. Instead, the experimental groups had to use remote laboratories in their respective departments. With the research building, IRIS Adlershof offers its members excellent working and teaching conditions thanks to 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.

Construction activity in the rear building section in 2016.
Deepest point: 13-meter excavation for the foundation of the NION-TEM.

IRIS Research Building fosters IRIS' integrative concept

The IRIS research building comprises 2500 m² of laboratory space, 2200 m² of office space, and several common rooms. In its core, the building offers laboratories of varying 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 labs. 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 adjacent to 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 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 discussions, presentations, and lectures. The entrance area itself is designed to provide space for poster presentations, which makes this building very suitable for conferences. The structure of the new research building thus reflects the interdisciplinary approach of IRIS Adlershof on the one hand and promotes interdisciplinary collaboration and communication on the other.

Setting up the joint lab in 2018

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 research building offers devices for photo- and electron beam-lithography within the cleanroom, a 19 m long glovebox cluster, an ultra-

Grand opening of the research building in October 2022.
From left to right: N. Puhlmann, J.P. Rabe, C. Markschies, U. Gote, J. von Blumenthal, C. Tischendorf, C. Schneider; Background: N. Helle-Meyer

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.

5. Selected Scientific Events

An important platform for communicating scientific results from IRIS Adlershof were the joint colloquia with the cooperation partners working on IRIS research project topics. The IRIS research areas of main interest in the collaborative research centers CRC 647, CRC 951, and CRC 1109 deserve special mention here.

In addition, IRIS Adlershof has organized further scientific events, which were coordinated or significantly influenced by IRIS Members. A selection can be found here:

5.1. IRIS Symposia

Symposium IRIS 2010: Systems for Optics and Electronics

July 12-14, 2010

Jürgen P. Rabe and William R. Salaneck

IRIS Adlershof was officially opened on July 12, 2010, in the presence of the then President of Humboldt-Universität zu Berlin, Prof. Christoph Markschies.

Following the opening ceremony, the "*1st International Symposium on Hybrid Systems for Optics and Electronics*" took place on July 13 and 14, 2010, where internationally renowned scientists presented the latest results in the field of hybrid materials research.

Symposium IRIS 2015: Chemistry & Physics of Macromolecules

November 20, 2015

Macromolecules, the dominating source in nature, play also a crucial role in a wide variety of industries. Natural Sciences are the key to analyse and understand their complex properties, which are unachievable by other materials, and design more and more specialised molecules and systems for further applications. The symposium is intended to feature a few but fine selected presentations on cutting-edge research on the physics and chemistry of functional (macro-)molecules.

IRIS-Manager Nikolai Puhlmann and Matthias Ballauff

Symposium IRIS 2017

June 29, 2017

The IRIS Symposium has firmly established itself as an annual highlight in the scientific life of IRIS Adlershof. It has also garnered growing interest beyond the Adlershof location, as evidenced by the annually increasing number of participants. The annual symposium aims to explore and discuss ideas for the further development of the Integrative Research Institute for the Sciences.

Oliver Benson during Symposium IRIS 2017

The IRIS 2017 Symposium focused on topics such as Charge Density Control, Analytical Sciences, Matters of Computation, and Matters of Activity. These topics were presented to an open-minded audience of internationally renowned researchers and business representatives.

Symposium IRIS 2018

June 21, 2018

The IRIS 2018 Symposium centered on ideas for the enhancement of Advanced Microscopy, Hybrid Materials for Optics and Electronics, Mathematical Physics of Complex Systems, and Quantum Technologies. To give young scientists the opportunity to present their research results to the invited speakers and symposium participants, IRIS introduced a poster competition in 2018. Laura Orphal received the Best Poster Award and a book voucher from IRIS Director Jürgen P. Rabe at the end of the symposium.

Eva Unger, Jürgen P. Rabe & HU's then Vice President for Research Peter Frensch

5.2. International conferences

CRC 951 Kick-Off meeting

December 14-16, 2011

On the occasion of its founding, the CRC 951 HIOS held a kick-off meeting from December 14 to 16, 2011, with the goal of discussing current research results in the field of inorganic/organic hybrid systems.

The following topics were comprehensively discussed:

- Synthesis and growth of hybrid structures and their components
- Electronic structure and energy level adjustment
- Optical properties, including charge carrier and exciton dynamics
- Optoelectronic/photonic functions and devices

7th International Symposium on Photochromism (ISOP) 2013

September 23–26, 2013

The ISOP series is a string of triannual events that are hosted on different continents and showcase the breadth of research on (organic) photochromism. After the very successful last two symposia 2007 in Vancouver and 2010 in Yokohama, this event carried on the tradition in Berlin in 2013 and highlighted the most recent results and trends in the burgeoning area of photochromism research. The symposium gathered the world's leading experts in the field and covered all aspects from the design of photochromic molecular systems all the way to their utilization in photoactive materials and photoswitchable biological tools. The symposium finished up with a one-day meeting of the PHENICS network to further strengthen the international collaboration on this topic and especially provide an additional opportunity for young researchers to present their research.

ERC-Grantees Conference 2014:
Frontiers in Chemistry – The Basis for Advanced Materials

August 28-29, 2014

The aim of the conference was to gather some of the leading European experts in the field of chemical materials research, showcase their latest achievements, and discuss future trends. For this purpose, around 20 ERC laureates (starting, consolidating, and advanced grants) active in the field of chemistry of materials were invited. Among them, there were two plenary lectures delivered by Klaus Müllen and Markus Antonietti, both leading figures in their generation of materials chemists.

The meeting aimed at providing a platform for young researchers to learn first-hand about the ERC granting schemes and creating a great opportunity to network and foster future collaborations within the European research landscape.

International Fπ14 Symposium

June 2-7, 2019

The Fπ symposium is a biennial international event dedicated to diverse aspects of functional materials with π-electrons. Over the years, the Fπ symposium has become one of the major conferences in the area of organic optoelectronics and related fields, gathering researchers from all over the world to share their latest results and to promote networking among the participants. It has been held only three times in Europa before.

IRIS Adlershof jointly organized the 14th International Symposium of Functional π-Electron Systems together with the HZB in Adlershof. The scientific program was co-organized by the IRIS Members Stefan Hecht and Norbert Koch. It was a further significant impulse for the international recognition of IRIS Adlershof and the importance of the Science and Technology Park Adlershof as a place for excellent research.

A total of over 500 participants were welcomed and important contacts were made for follow-up discussions.

5.3. Summer schools and junior workshops

KOSMOS Summer University 2011: Frontiers of Organic/ Inorganic Hybrid Materials for Electronics and Optoelectronics

September 17-25, 2011

The first KOSMOS Summer University of Humboldt-Universität zu Berlin, KOSMOS 2011, was held from September 17 to 25, 2011, organized by IRIS Adlershof in collaboration with Chiba University and the National University of Singapore. Master's students in their final phase, doctoral candidates, and postdocs worked together with internationally renowned researchers in the physics and chemistry of hybrid materials to develop a fundamental understanding of this promising class of new materials.

KOSMOS Summer University 2014:
Chemistry and Physics of Novel Materials for (Opto-) Electronics

July 8-19, 2014

The main goal of this Summer University was to teach the fundamentals of (opto)electronic materials through an integrative approach, combining expertise in the 'three Ms': Make, Measure, and Model. Organized in cooperation with the National University of Singapore and Princeton University, it brought together young researchers from diverse backgrounds for a creative, interactive learning experience. The program included tutorials, research highlights by field leaders, literature analysis, and the development of innovative ideas in interdisciplinary teams.

Stefan Hecht discusses with participants of the Summer University

Humboldt-Princeton Exchange Workshop on Novel Opto-Electronic Materials

October 27-28, 2013

The future progress of our information-based society demands the concentration of optoelectronic functions with increasingly higher capabilities in smaller and smaller volumes. At the same time, the steadily increasing mobility of individuals and the need for a reliable flow of high-volume data call for lightweight devices with mechanical flexibility, such as in smart clothing. Yet another pressing challenge is the efficient generation of energy from renewable sources, such as photovoltaics, which needs to become available in substantial quantities in the short term. Established materials have been pushed close to their intrinsic limits, and many of the devices and systems using these materials are not lightweight or bendable (e.g., silicon-based electronics). Furthermore, the primary energy required for the fabrication of presently established technologies is significant and could be reduced by developing new, appropriate materials and production methods. Organic and hybrid organic/inorganic material combinations offer a way to overcome some of the current limitations.

The fields of organic electronics and optoelectronics have seen considerable advances in the past decade, with remarkable progress in light emission or harvesting, flexible electronics, and sensors.

Some of these applications are already successfully penetrating the market. Hybrid materials for optoelectronic applications are at a comparatively early research stage. Both material classes, organic and hybrid materials, offer the possibility for direct printing from solution, which could enable large-scale, low-cost fabrication of electronic and optoelectronic components and devices in a roll-to-roll (R2R) fashion. Further progress in this area critically depends on intensive research efforts on organic and hybrid semiconductor materials with a strong focus on material chemistry, electronic structure, mechanical properties, and device integration.

Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence - A Workshop and Hands-on Tutorial.

July 25–29, 2022

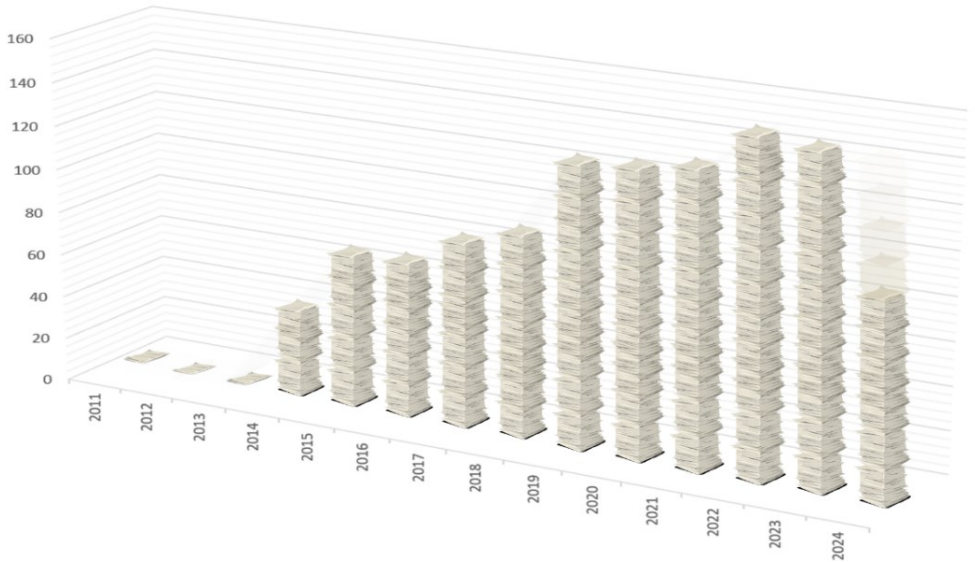
The first summer school, organized by IRIS Adlershof in collaboration with the Pritzker School of Molecular Engineering (University of Chicago), was held in summer 2022 at HU's science campus in Adlershof. The event was titled: Modeling Materials at Realistic Time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence - A Workshop and Hands-on Tutorial. The scientific program was co-organized by the IRIS Member Matthias Scheffler.

During the first three days, from July 25th to 27th, leading experts from various fields gave talks on computational applications and related artificial intelligence methods in the context of 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 27th featured an excursion to a graffiti tour at Teufelsberg, followed by dinner.

The last two days were dedicated to tutorials with hands-on examples focusing on the simulation of molecular dynamics.

6. Publications and Scientific Highlights

Since 2009, IRIS Members have published over 2,500 works. IRIS Adlershof has evolved beyond just an academic network, as its members increasingly recognized it as an official institutional affiliation in their publications, reinforcing its standing within the scientific community, as shown in the graphic below.



Publications with the affiliation "IRIS Adlershof" per year , based on Scopus search, as of Sept. 2024

A list of publications is available at: *www.iris-adlershof.de/publications*. We feature the three most-cited publications to highlight our impact in the following list.

Throughout its history, IRIS Adlershof has experienced many significant moments, both large and small, which we have highlighted on our website since 2011. In the following list, we include one notable highlight from each year, aiming to showcase the diversity of our work rather than ranking our achievements.

2009

Density-functional calculations of the structure of near-surface oxygen vacancies and electron localization on CeO2(111)
M. V. Ganduglia-Pirovano, J. L. F. Da Silva, and J. Sauer
Physical Review Letters 102 (2009) 026101
DOI: 10.1103/PhysRevLett.102.026101

Conductance of a Single Conjugated Polymer as a Continuous Function of Its Length
L. Lafferentz, F. Ample, H. Yu, S. Hecht, C. Joachim, and L. Grill
Science 323 (2009) 1193
DOI: 10.1126/science.1168255

Plasmon-Enhanced Single Photon Emission from a Nanoassembled Metal–Diamond Hybrid Structure at Room Temperature
S. Schietinger, M. Barth, T. Aichele, and O. Benson
Nano Letters 9 (2009) 1694
DOI: 10.1021/nl900384c

2010

Kinetic Analysis of Catalytic Reduction of 4-Nitrophenol by Metallic Nanoparticles Immobilized in Spherical Polyelectrolyte Brushes
S. Wunder, F. Polzer, Y. Lu, Y. Mei, and M. Ballauff
J. Phys. Chem. C 114 (2010) 8814
DOI: 10.1021/jp101125j

Photoswitches: From Molecules to Materials
M.-M. Russew and S. Hecht
Adv. Mater. 22 (2010) 3348
DOI: 10.1002/adma.200904102

Plasmon-Enhanced Upconversion in Single $NaYF_4:Yb^{3+}/Er^{3+}$ Codoped Nanocrystals
S. Schietinger, T. Aichele, H-Q. Wang, T. Nann, and O. Benson
Nano Letters 10 (2010) 134
DOI: 10.1021/nl903046r

2011

Catalytic Activity of Faceted Gold Nanoparticles Studied by a Model Reaction: Evidence for Substrate-Induced Surface Restructuring
S. Wunder, Y. Lu, M. Albrecht, and M. Ballauff
ACS Catalysis 1 (2011) 908
DOI: 10.1021/cs200208a

Ultrafast nonequilibrium carrier dynamics in a single graphene layer
M. Breusing, S. Kuehn, T. Winzer, E. Malić, F. Milde, N. Severin, J. P. Rabe, C. Ropers, A. Knorr, and T. Elsaesser
Phys. Rev. B 83 (2011) 153410
DOI: 10.1103/PhysRevB.83.153410

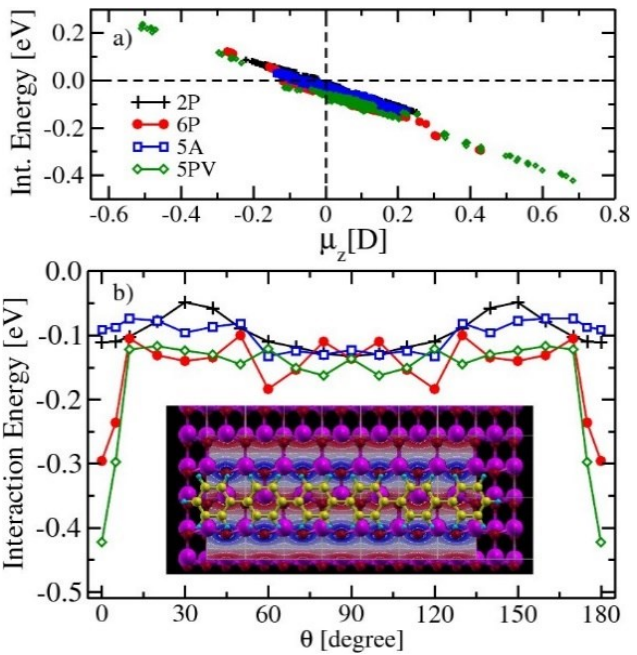
Assembly of hybrid photonic architectures from nanophotonic constituents
O. Benson
Nature 480 (2011) 193
DOI: 10.1038/nature10610

Electrostatic-Field Driven Alignment of Organic Oligomers on ZnO Surface

The physisorption of organic oligomers on the strongly ionic ZnO(1010) surface has been studied by Fabio della Sala (NNL, Lecce), Sylke Blumstengel, and Fritz Henneberger (both IRIS Adlershof and Department of Physics HU Berlin). In previous experiments (see S. Blumstengel et al., Phys. Chem. Chem. Phys. 12, (2010) 11642), it has been found that sexiphenyl adsorbs on this surface in a well-defined orientation where the long axis of the flat-lying molecules is aligned perpendicular to the c-direction of the ZnO crystal. Using first-principles density-functional theory and non-empirical embedding methods, it could be demonstrated that this observation is representative of a generic scenario related to the strong dipolar electrostatic field created by the ZnO surface dimers. The electrostatic molecule-substrate coupling is characterized by a linear relation between the in-plane variation of the interaction energy and the molecular dipole moment induced in vertical direction. Long oligomers with a highly axial π-electron system are aligned along rows of positive electric field. The energies required for reorientation reach some 100 meV. These findings define a new route

towards the realization of highly ordered self-assembled arrays of oligomers/polymers on inorganic semiconductors as well as for the interfacial energy level adjustment.

F. Della Sala, S. Blumstengel, &
F. Henneberger
Electrostatic-field-driven alignment of organic oligomers on ZnO surfaces.
Physical Review Letters, 107(14), 146401.
DOI: 10.1103/PhysRevLett.107.146401



Electrostatic molecule-substrate interaction energy for biphenyle (2P), sexiphenyl (6P), pentacene (5A), and penta-phenylene-vinylene(5PV) on ZnO(1010).
a) Linear relation between the interaction energy and the molecular dipole moment μz induced in vertical direction.
b) Interaction energy versus rotation angle Θ.
Inset: Orientation of 6P at the global minimum shown on a colormap

2012

Catalysis by metallic nanoparticles in aqueous solution: model reactions
P. Hervés, M. Pérez-Lorenzo, L. M. Liz-Marzán, J. Dzubiella, Y. Lu, and M. Ballauff
Chem. Soc. Rev. 41 (2012) 5577
DOI: 10.1039/C2CS35029G

Review of AdS/CFT Integrability: An Overview
N. Beisert, C. Ahn, L. F. Alday, Z. Bajnok, J. M. Drummond, L. Freyhult, N. Gromov, R. A. Janik, V. Kazakov, T. Klose, G. P. Korchemsky, C. Kristjansen, M. Magro, T. McLoughlin, J. A. Minahan, R. I. Nepomechie, A. Rej, R. Roiban, S. Schäfer-Nameki, C. Sieg, M. Staudacher, A. Torrielli, A. A. Tseytlin, P. Vieira, D. Volin, and K. Zoubos
Lett. Math. Phys. 99 (2012) 3
DOI: 10.1007/s11005-011-0529-2

Multivalency as a Chemical Organization and Action Principle
C. Fasting, C. A. Schalley, M. Weber, O. Seitz, S. Hecht, B. Koksch, J. Dernedde, C. Graf, E.-W. Knapp, and R. Haag
Angew. Chem. Int. Ed. 51 (2012) 10472
DOI: 10.1002/anie.201201114

Organic Thin-Film Transistors Adressable by Light

Organic semiconductors are key components for the development of printable, flexible, and large-area electronics. To realize complex device functions the materials should exhibit several (meta-stable) states, between which can be switched selectively with different stimuli ("addressing"). Amongst possible stimuli, light is very attractive as it provides unprecedented spatio-temporal control and can be easily interfaced with advanced optics. However, in order to introduce light-responsiveness in organic devices photo-switchable molecular building blocks have to be incorporated into the material, ideally in a convenient and practical process. An international research team including Stefan Hecht and Norbert Koch – both members of IRIS Adlershof – has now realized such “smart“ transistors that can be addressed by light. As described in their article in Nature Chemistry the authors demonstrated a new concept by introducing photo-switchable electron-hole traps into the active layer of the device. These specifically designed small molecules are able to interfere with the charge flow through the transistor’s semiconducting polymer in one particular state, which is generated by illumination with UV-light. Illumination with visible light disables the traps and re-establishes the initial state, in which charge flow is not affected (see Figure).

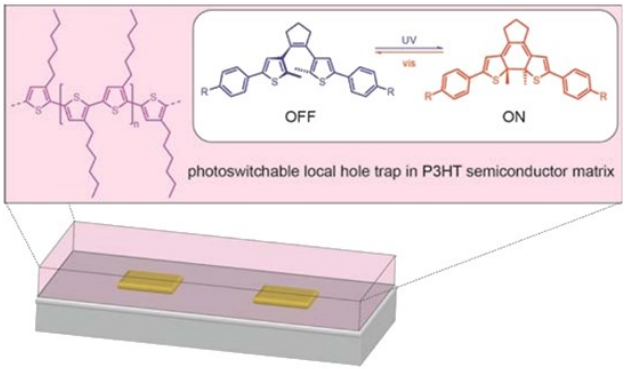


Figure: "Smart" transistors gated by light: UV-illumination transforms ring-open dithienylethene (blue) to its ring-closed isomer (red), which effectively traps holes in the semiconducting poly(3-hexylthiophene) (P3HT) matrix. Illumination with visible light reverts the process and reinstalls charge flow through the device.

The new method of simple blending of trap molecules with the semiconductor matrix is highly effective yet simple, and hence applicable to large-scale device fabrication processes. The light-programmable transistors could serve as multifunctional elements in logic circuits.

E. Orgiu, N. Crivillers, M. Herder, L. Grubert, M. Pätzel, J. Frisch, E. Pavlica, D. T. Duong, G. Bratina, A. Salleo, N. Koch, S. Hecht, P. Samorì
Organic Thin-Film Transistors Adressable by Light
Nature Chemistry 4 (2012) 675
DOI: 10.1038/nchem.1384

2013

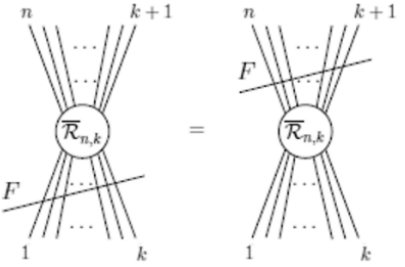
Oxygen Defects and Surface Chemistry of Ceria:
Quantum Chemical Studies Compared to Experiment
J. Paier, C. Penschke, and J. Sauer
Chemical Reviews 113 (2013) 3949
DOI: 10.1021/cr3004949

ElaStic: A tool for calculating second-order elastic constants from first principles
R. Golesorkhtabar, P. Pavon, J. Spitaler, P. Puschnig, and C. Draxl
Comput. Phys. Commun. 184 (2013) 1861
DOI: 10.1016/j.cpc.2013.03.010

Moderate doping leads to high performance of semiconductor/insulator polymer blend transistors
Guanghao Lu, J. Blakesley, S. Himmelberger, P. Pingel, J. Frisch, I. Lieberwirth, I. Salzmann, M. Oehzelt, R. Di Pietro, A. Salleo, N. Koch, and D. Neher
Nat. Commun. 4 (2013) 1588
DOI: 10.1038/ncomms2587

Spin Chain Techniques for Scattering Amplitudes in Quantum Field Theory

Jan Plefka and Matthias Staudacher (both IRIS Adlershof) applied the mathematical technique termed "integrability", which is borrowed from the exact solution of spin chain models in condensed matter theory, to the calculation of scattering amplitudes in four dimensional quantum Yang-Mills theory. The latter are a class of models used at particle physics colliders such as the LHC in Geneva to study matter at very small scales and high energies. In a joint work with postdoctoral researchers Livia Ferro and Tomasz Łukowski, as well as former student Carlo Meneghelli, the idea of introducing a so-called spectral parameter into the amplitude problem was born. The existence of this parameter is a hallmark of quantum integrability, as it appears in certain spin chain models and special Yang-Mills theories. The authors supplied initial evidence that the spectral parameter might find its use as a novel symmetry-respecting regulator for the vexing infrared divergences of the amplitudes. Its physical meaning is a local deformation of particle helicity, a fact that might be useful for a much larger class of non-integrable, realistic four-dimensional field theories.



A scattering amplitude of a gauge theory probed by a fictitious “test particle”. The resulting equation is a generalization of the so-called Yang Baxter equation appearing in the mathematical description of certain spin chains of condensed matter theory, as well as in some four dimensional quantum field theories.

L. Ferro, T. Łukowski, C. Meneghelli, J. Plefka, and M. Staudacher
Harmonic R Matrices for Scattering Amplitudes and Spectral Regularization
Phys. Rev. Lett. 110 (2013) 121602
DOI: 10.1103/PhysRevLett.110.121602

2014

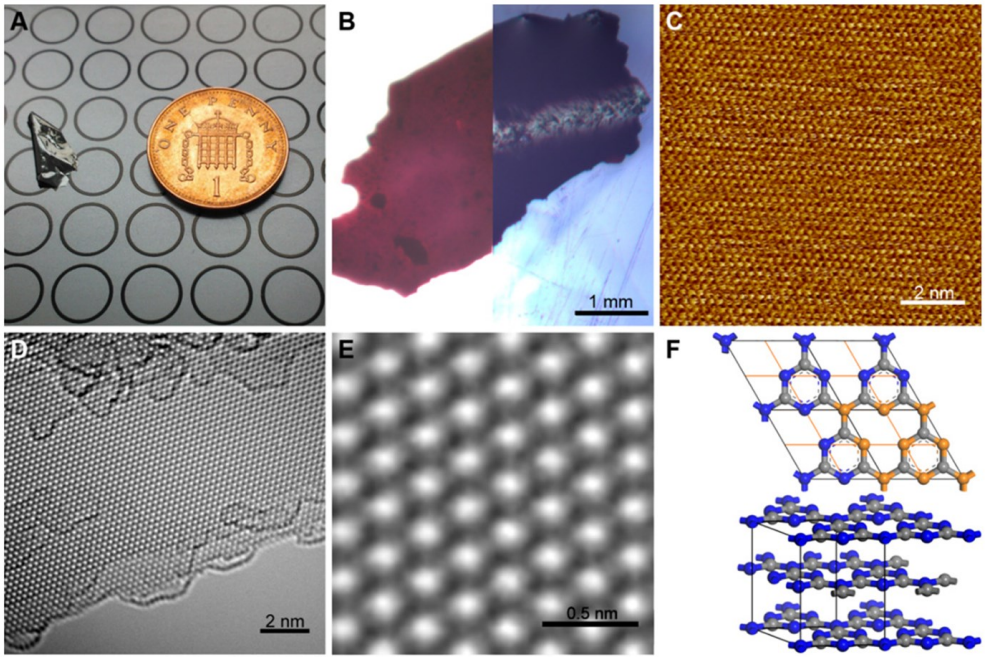
Protein Interactions with Polymer Coatings and Biomaterials
Q. Wei, T. Becherer, S. Angioletti-Uberti, J. Dzubiella, C. Wischke, A. T. Neffe, A. Lendlein, M. Ballauff, and R. Haag
Angew. Chem. Int. Ed. 53 (2014) 8004
DOI: 10.1002/anie.201400546

Triazine-Based Graphitic Carbon Nitride: a Two-Dimensional Semiconductor
G. Algara-Siller, N. Severin, S. Y. Chong, T. Björkman, R. G. Palgrave, A. Laybourn, M. Antonietti, Y. Z. Khimyak, A. V. Krasheninnikov, J. P. Rabe, U. Kaiser, A. I. Cooper, A. Thomas, and M. J. Bojdys
Angew. Chem. Int. Ed. 53 (2014) 7450
DOI: 10.1002/anie.201402191

The Stratosphere platform for big data analytics
A. Alexandrov, R. Bergmann, S. Ewen, J.-C. Freytag, F. Hueske, A. Heise, O. Kao, M. Leich, U. Leser, V. Markl, F. Naumann, M. Peters, A. Rheinländer, M. J. Sax, S. Schelter, M. Höger, K. Tzoumas, and D. Warneke
The VLDB Journal 23 (2014) 939
DOI: 10.1007/s00778-014-0357-y

Long sought two-dimensional graphitic semiconductor discovered

A European team of chemists and physicists, including Nikolai Severin and Jürgen P. Rabe of the Department of Physics of Humboldt-Universität and the Joint Laboratory of Structural Research at IRIS Adlershof, have discovered a new quasi two-dimensional semiconductor related to graphene (see comment in ars technica). The novel material, 'triazine-based graphitic carbon nitride' (TGCN) was predicted theoretically in 1996, but this is the first time that it has been presented. TGCN is a member of the graphene family, of which only five non-metallic 2D materials were known up to date: graphene itself, hexagonal boron nitride, boron carbon nitride, fluorographene and graphene oxide. TGCN is structurally similar to graphite but a semiconductor, which is of high interest for opto-electronic applications.



Physical characterization of TGCN. A) Single macroscopic flake. B) Optical microscopy images in transmission (left half) and reflection (right half). C–E) Mechanically cleaved layers as imaged by SFM (C) and by HR-TEM (D and E). F) Crystallographic unit cell and AB stacking arrangement of TGCN layers derived from structural refinement.

Cooperation partners in this project are Michael J. Bojdys and Arne Thomas (TU Berlin), Markus Antonietti (MPI of Colloids and Interfaces) and five further groups from the UK, Germany and Finland. Within IRIS Adlershof 2D atomic crystals play an important role in the Research Area "Hybrid Systems for Optic and Electronics".

G. Algara-Siller, N. Severin, S.Y. Chong, T. Björkman, R.G. Palgrave, A. Laybourn, M. Antonietti, Y.Z. Khimyak, A.V. Krasheninnikov, J.P. Rabe, U. Kaiser, A.I. Cooper, A. Thomas, and M.J. Bojdys
Triazine-Based Graphitic Carbon Nitride: a Two-Dimensional Semiconductor
Angew. Chem. 126 (2014) 7580 // DOI: 10.1002/ange.201402191
Angew. Chem. Int. Ed. 53 (2014) 7450 // DOI: 10.1002/anie.201402191

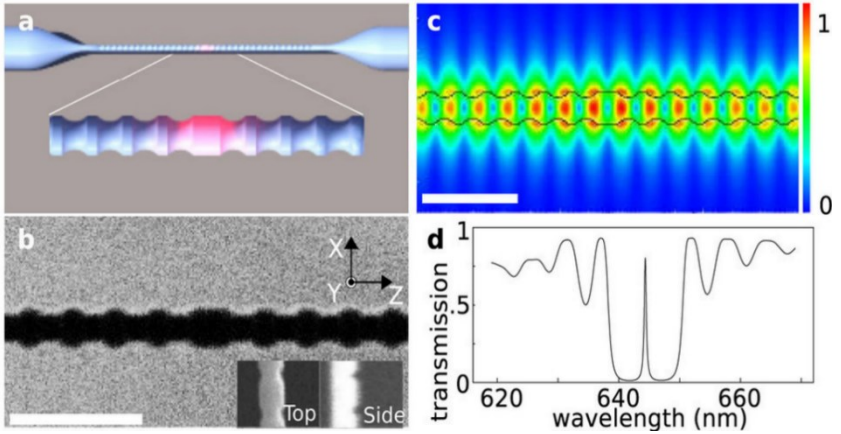
2015

Big Data of Materials Science: Critical Role of the Descriptor
L. M. Ghiringhelli, J. Vybiral, S. V. Levchenko, C. Draxl, and M. Scheffler
Phys. Rev. Lett. 114 (2015) 105503
DOI: 10.1103/PhysRevLett.114.105503

Visible-Light-Activated Molecular Switches
D. Bléger and S. Hecht
Chem. Int. Ed. 54 (2015) 11338
DOI: 10.1002/anie.201500628

Charge-transfer crystallites as molecular electrical dopants
H. Méndez, G. Heimel, S. Winkler, J. Frisch, A. Opitz, K. Sauer, B. Wegner, M. Oehzelt, C. Röthel, S. Duhm, D. Többens, N. Koch, and I. Salzmann
Nat. Commun. 6 (2015) 8560
DOI: 10.1038/ncomms9560

More Photons Through an Optical Nanofiber



a) Sketch of a structured nanofiber
b) Scanning ion microscope image of a nanofiber (diameter 270 nm, groove depth 45 nm, groove spacing 300 nm, and defect length 450 nm)
c) Electric field, numerically calculated. The black line indicates the cavity structure
d) Calculated transmission spectrum.

An international team of researchers from Humboldt-Universität zu Berlin, led by Oliver Benson, a member of IRIS Adlershof, and researchers from Kyoto University in Japan, has succeeded in enhancing the emission of single light particles, known as photons, using an innovative structured nanofiber. The experiment not only produced an extraordinarily large number of photons, but also

allowed their wavelength to be precisely adjusted. These custom-tailored photons can be directly utilized for applications in new quantum technologies via the fiber. The research results have been published in the Open-Access journal “Scientific Reports”.

The structured nanofiber is a special type of microresonator, which is used to investigate fundamental physical effects in the field of quantum optics. Similar to how a tuning fork stores sound waves, microresonators store light of a certain wavelength for a very long time and further amplify it. Interactions between photons and the smallest quantities of matter - down to a single atom - can thus be controlled, enhanced, and utilized. To produce the microresonators, the researchers used a focused beam of gallium ions to engrave tiny structures onto a glass fiber that is only a few hundred nanometers thick. This diameter is more than a hundred times smaller than that of a human hair. Tiny semiconductor crystals, just a few nanometers in size, served as photon sources. These crystals were precisely placed on the structured region of the nanofiber. As a result, the light emission was amplified, and photons were emitted directly into the glass fiber.

A microresonator can only store and amplify light of a specific wavelength. If this light is to be coupled with certain molecules or atoms, for example, for molecular or atomic optical switches, the resonator must be precisely tuned. The researchers succeeded in this by using a simple mechanism: by stretching the nanofiber, they were able to controllably deform it and thus change the properties of

the resonator as needed. In a system with many different switching elements, these can be aligned with each other. This targeted interaction would form the basis for an integrated optical quantum chip, which is required for quantum computing on quantum computers.

Currently, the researchers are working on further improving the microresonators and coupling them with other optical emitters in addition to semiconductor crystals. This would expand the range of possible applications, for example, in telecommunications for secure data transmission through quantum cryptography. Furthermore, a single molecule coupled to the fiber could be used as a nanosensor. Such a sensor would be the smallest possible and could detect minuscule amounts of substances with unprecedented accuracy.

A. W. Schell, H. Takashima, S. Kamioka, Y. Oe, M. Fujiwara, O. Benson, and S. Takeuchi
Highly Efficient Coupling of Nanolight Emitters to an Ultra-Wide Tunable Nanofibre Cavity
Sci. Rep. 5 (2015) 9619
DOI: 10.1038/srep09619

2016

Nanostructured Materials for Room-Temperature Gas Sensors
J. Zhang, X. Liu, G. Neri, and N. Pinna
Adv. Mater. 28 (2016) 795
DOI: 10.1002/adma.201503825

Reproducibility in density functional theory calculations of solids
K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dułak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier

Science 351 (2016) aad3000
DOI: 10.1126/science.aad3000

Molecular Electrical Doping of Organic Semiconductors: Fundamental Mechanisms and Emerging Dopant Design Rules
I. Salzmann, G. Heimel, M. Oehzelt, S. Winkler, and N. Koch
Acc. Chem. Res. 49 (2016) 370
DOI: 10.1021/acs.accounts.5b00438

Reproducibility in density functional theory calculations of solids

The success and widespread popularity of density functional theory (DFT) over the last decades has given rise to an extensive range of dedicated codes for predicting molecular and crystalline properties. However, each code implements the formalism in a different way, raising questions about the reproducibility of such predictions. In this article, the results of a community-wide effort is reported, comparing 15 solid-state codes, using 40 different potentials or basis set types, to assess the quality of the equations of state for 71 elemental crystals.

The overall conclusion is that predictions from recent codes and pseudopotentials agree very well, with pairwise differences that are comparable to those between different high-precision experiments. Results of older methods, however, show stronger discrepancies.

exciting, the program package [1,2] developed in the group of Claudia Draxl at Humboldt-Universität zu Berlin (Physics Department and IRIS Adlershof) represents one of the all-electron full-potential implementations of DFT. It employs the linearized-augmented planewave basis, which is considered the gold standard within the condensed matter community. Within this study, exciting has proven to be among the three most precise packages, with nearly negligible differences between them. exciting has not only evolved into a benchmark code for DFT but has a strong focus on excitations that are treated within time-dependent DFT and many-body perturbation theory. In August 2016, HoW exciting! 2016 [3] took place at the Campus Adlershof, consisting of an international workshop on excitations in solids and a hands-on course employing exciting.

[1] exciting-code.org

[2] exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory
A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, C. Draxl

J. Phys: Condes. Matter (Topical Review) 26 (2014) 363202
DOI: 10.1088/0953-8984/26/36/363202

[3] how-exciting-2016.physik.hu-berlin.de

Reproducibility in density functional theory calculations of solids
K. Lejaeghere, *et al.* (Full author list on p. 82)
Science 351 (2016), 1415
DOI: 10.1126/science.aad3000

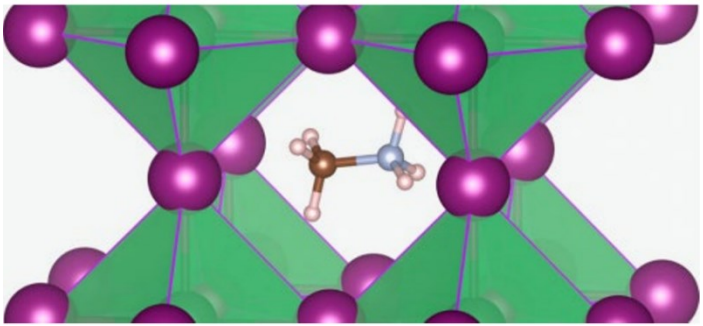
2017

Two-Dimensional Nanostructured Materials for Gas Sensing
X. Liu, T. Ma, N. Pinna, and J. Zhang
Adv. Funct. Mater. 27 (2017) 1702168
DOI: 10.1002/adfm.201702168

Water Dynamics in the Hydration Shells of Biomolecules
D. Laage, T. Elsaesser, and J. T. Hynes
Chemical Reviews 117 (2017) 10694
DOI: 10.1021/acs.chemrev.6b00765

Large guanidinium cation mixed with methylammonium in lead iodide perovskites for 19% efficient solar cells
A. D. Jodlowski, C. Roldán-Carmona, G. Grancini, M. Salado, M. Ralaiarisoa, S. Ahmad, N. Koch, L. Camacho, G. de Miguel, M. K. Nazeeruddin
Nat Energy 2 (2017) 972
DOI: 10.1038/s41560-017-0054-3

Longer lifetimes for perovskite absorber



An international team of scientists has improved greatly the stability of organic-inorganic lead halide perovskites. These materials have enormous potential for photovoltaic applications but still suffer from comparably moderate device lifetime. The scientists, led by researchers from the EPFL, Lausanne, Switzerland, incorporated a large organic cation – guanidinium - into the perovskite crystal structure, in part replacing the traditionally used methylammonium and formamidinium cations. Overall, the new material delivered average power conversion efficiencies over 19%, and stabilized performance for 1,000 h under continuous light illumination. This is a fundamental step within the perovskite field. These groundbreaking research results were published in Nature Energy. Among the authors is Norbert Koch, who is a member of IRIS Adlershof.

Large guanidinium cation mixed with methylammonium in lead iodide perovskites for 19% efficient solar cells

A.D. Jodlowski, C. Roldán-Carmona, G. Grancini, M. Salado, M. Ralaiarisoa, S. Ahmad, N. Koch, L. Camacho, G. de Miguel, and M.K. Nazeeruddin

Nature Energy 2 (2017) 972-979

DOI: 10.1038/s41560-017-0054-3

2018

NOMAD: The FAIR concept for big data-driven materials science
C. Draxl and M. Scheffler
MRS Bulletin 43 (2018) 676
DOI: 10.1557/mrs.2018.208

Carbon nitride supported Fe2 cluster catalysts with superior performance for alkene epoxidation
S. Tian, Q. Fu, W. Chen, Q. Feng, Z. Chen, J. Zhang, W.-C. Cheong, R. Yu, L. Gu, J. Dong, J. Luo, C. Chen, Q. Peng, C. Draxl, D. Wang, and Y. Li
Nat Commun 9 (2018) 2353
DOI: 10.1038/s41467-018-04845-x

Influence of Charge Transport Layers on Open-Circuit Voltage and Hysteresis in Perovskite Solar Cells
S. Ravishankar, S. Gharibzadeh, C. Roldán-Carmona, G. Grancini, Y. Lee, M. Ralaiarisoa, A. M. Asiri, N. Koch, J. Bisquert, and M. K. Nazeeruddin
Joule 2 (2018) 788
DOI: 10.1016/j.joule.2018.02.013

SPACE – TIME – MATTER: Analytic and Geometric Structures

Jochen Brüning,
Matthias Staudacher (Eds.)

SPACE – TIME – MATTER:
Analytic and Geometric
Structures

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This monograph describes some of the most interesting results obtained by the mathematicians and physicists collaborating in the *CRC 647 Space-Time-Matter*, in the years 2005 – 2016. It concerns the mathematical and physical foundations of string and quantum field theory as well as cosmology. The work starts with an excellent introduction by the editors Jochen Brüning and Matthias Staudacher, that gives an historical overview of the field and vividly retells the development of the CRC. Then each project of the final funding period is summarized and also represented in detail by the following 15 chapters, many contributed by IRIS scientists:

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

2019

The impact of energy alignment and interfacial recombination on the internal and external open-circuit voltage of perovskite solar cells
M. Stolterfoht, P. Caprioglio, C. M. Wolff, J. A. Márquez, J. Nordmann, S. Zhang, D. Rothhardt, U. Hörmann, Y. Amir, A. Redinger, L. Kegelmann, F. Zu, S. Albrecht, N. Koch, T. Kirchartz, M. Saliba, T. Unold, and D. Neher
Energy Environ. Sci., 12 (2019) 2778
DOI: 10.1039/C9EE02020A

Ni Strongly Coupled with Mo2C Encapsulated in Nitrogen-Doped Carbon Nanofibers as Robust Bifunctional Catalyst for Overall Water Splitting
M. Li, Y. Zhu, H. Wang, C. Wang, N. Pinna, and X. Lu
Adv. Energy Mater. 9 (2019) 1803185
DOI: 10.1002/aenm.201803185

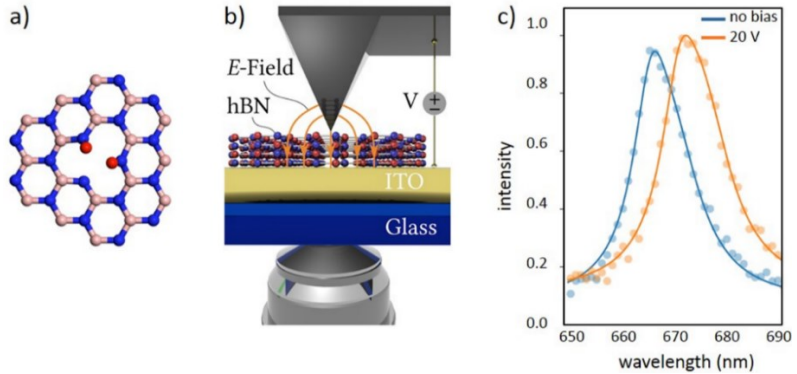
Surface Termination Dependent Work Function and Electronic Properties of Ti3C2Tx MXene
T. Schultz, N. C. Frey, K. Hantanasirisakul, S. Park, S. J. May, V. B. Shenoy, Y. Gogotsi, and N. Koch
Chemistry of Materials 31 (2019) 6590
DOI: 10.1021/acs.chemmater.9b00414

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

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

Based on their results the researchers suggest building a room-temperature single photon source, which can be tuned electrically in or out of a resonance of a plasmonic resonator. "Such a source would be highly desirable as a reliable non-classical light source for applications in quantum-

enhanced sensing and metrology or in quantum key distribution." says Oliver Benson, who is researcher in IRIS Adlershof and leads the Humboldt-team.



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

Very large and Reversible Stark-Shift Tuning of Single Emitters in Layered Hexagonal Boron Nitride
N. Nikolay, N. Mendelson, N. Sadzak, F. Böhm, T. T. Tran, B. Sontheimer, I. Aharonovich, and O. Benson
Phys. Rev. Applied 11 (2019) 041001, DOI: 10.1103/PhysRevApplied.11.041001

2020

Polymer-Derived Heteroatom-Doped Porous Carbon Materials
H. Wang, Y. Shao, S. Mei, Y. Lu, M. Zhang, J.-k. Sun, K. Matyjaszewski, M. Antonietti, and J. Yuan
Chemical Reviews 120 (2020) 9363
DOI: 10.1021/acs.chemrev.0c00080

Hybrid integrated quantum photonic circuits
A. W. Elshaari, W. Pernice, K. Srinivasan, O. Benson, and V. Zwiller
Nat. Photonics 14 (2020) 285
DOI: 10.1038/s41566-020-0609-x

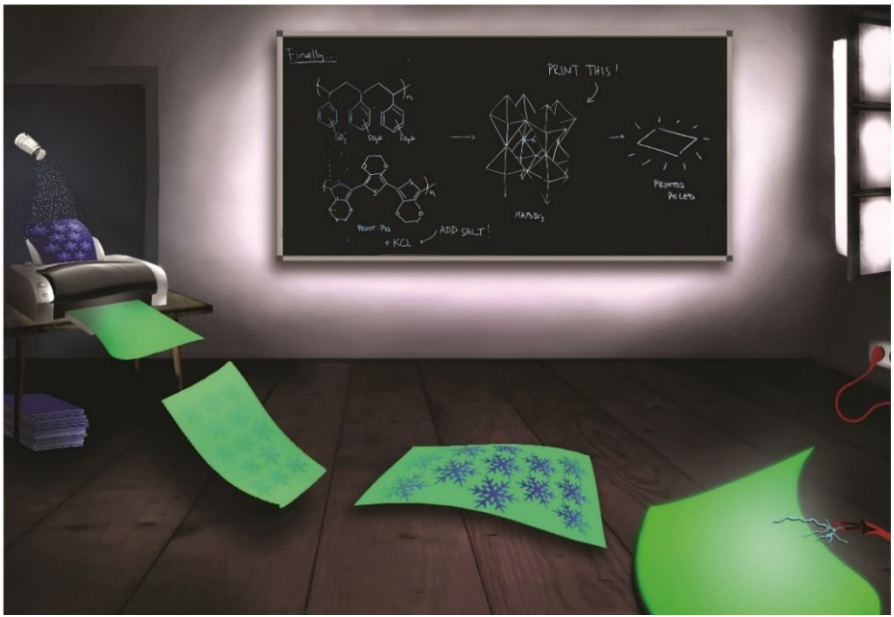
Enlightening Materials with Photoswitches
A. Goulet-Hanssens, F. Eisenreich, and S. Hecht
Adv. Mater. 32 (2020) 1905966
DOI: 10.1002/adma.201905966

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

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

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

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



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

Scientists at HZB have already shown in recent years that solar cells can be printed from a solution of semiconductor compounds – and are worldwide leaders in this technology today. Now for the first time, the joint team of HZB and HU Berlin has succeeded in producing functional light-emitting diodes in this manner. The research group used a metal halide perovskite for this purpose. This is a material that promises particularly high efficiency in generating light – but on the other hand is difficult to process. “Until now, it has not been possible to produce these kinds of semiconductor layers with sufficient quality from a liquid solution“, says List-Kratochvil. For example, LEDs could be printed just from organic semiconductors, but these provide only modest luminosity. “The challenge was how to cause the salt-like precursor that we printed onto the substrate to crystallise quickly and evenly by using some sort of an attractant or catalyst“, explains the scientist. The team chose a seed crystal for this purpose: a salt crystal that attaches itself to the substrate and triggers formation of a gridwork for the subsequent perovskite layers.

In this way, the researchers created printed LEDs that possess far higher luminosity and considerably better electrical properties than could be previously achieved using additive manufacturing processes. But for List-Kratochvil, this success is only an intermediate step on the road to future micro- and optoelectronics that he believes will be based exclusively on hybrid perovskite semiconductors. “The advantages offered by a single universally applicable class of materials and a single cost-effective and simple process for manufacturing any kind of component are striking“, says

the scientist. He is therefore planning to eventually manufacture all important electronic components this way in the laboratories of HZB and HU Berlin.

Finally, inkjet-printed metal halide perovskite LEDs – utilizing seed crystal templating of salty PEDOT:PSS
F. Hermerschmidt, F. Mathies, V.R.F. Schröder, C. Rehermann, N. Zorn Morales, E.L. Unger, E.J.W. List-Kratochvil
Mater. Horiz., 2020,7, 1773
DOI: 10.1039/D0MH00512F

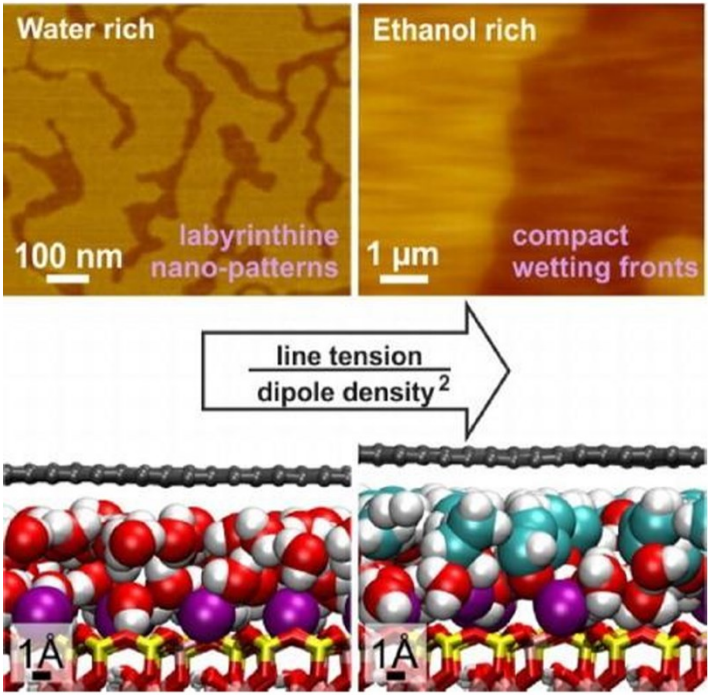
2021

Protonated Imine-Linked Covalent Organic Frameworks for Photocatalytic Hydrogen Evolution
J. Yang, A. Acharjya, M.-Y. Ye, J. Rabeah, S. Li, Z. Kochovski, S. Youk, J. Roeser, J. Grüneberg, C. Penschke, M. Schwarze, T. Wang, Y. Lu, R. van de Krol, M. Oschatz, R. Schomäcker, P. Saalfrank, and A. Thomas
Angew. Chem. Int. Ed. 60 (2021) 19797
DOI: 10.1002/anie.202104870

20.8% Slot-Die Coated MAPbI3 Perovskite Solar Cells by Optimal DMSO-Content and Age of 2-ME Based Precursor Inks
J. Li, J. Dagar, O. Shargaieva, M. A. Flatken, H. Köbler, M. Fenske, C. Schultz, B. Stegemann, J. Just, D. M. Többens, A. Abate, R. Munir, and E. Unger
Adv. Energy Mater. 11 (2021) 2003460
DOI: 10.1002/aenm.202003460

Recent Advances in Multimetal and Doped Transition-Metal Phosphides for the Hydrogen Evolution Reaction at Different pH values
S. M. El-Refaei, P. A. Russo, and N. Pinna
ACS Applied Materials & Interfaces 13 (2021) 22077
DOI: 10.1021/acsami.1c02129

Shaping 2D materials with small molecules



Scanning force microscopy images of graphene surfaces shaped by an intercalating molecularly thin water layer selfassembled 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.

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 group of Jürgen P. Rabe 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

2022

Doping Approaches for Organic Semiconductors
A. D. Scaccabarozzi, A. Basu, F. Aniés, J. Liu, O. Zapata-Arteaga, R. Warren, Y. Firdaus, M. I. Nugraha, Y. Lin, M. Campoy-Quiles, N. Koch, C. Müller, L. Tsetseris, M. Heeney, and T. D. Anthopoulos
Chem. Rev. 122 (2022) 4420
DOI: 10.1021/acs.chemrev.1c00581

Nano-optical designs for high-efficiency monolithic perovskite–silicon tandem solar cells
P. Tockhorn, J. Sutter, A. Cruz, P. Wagner, 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
Nat. Nanotechnol. 17 (2022) 1214
DOI: 10.1038/s41565-022-01228-8

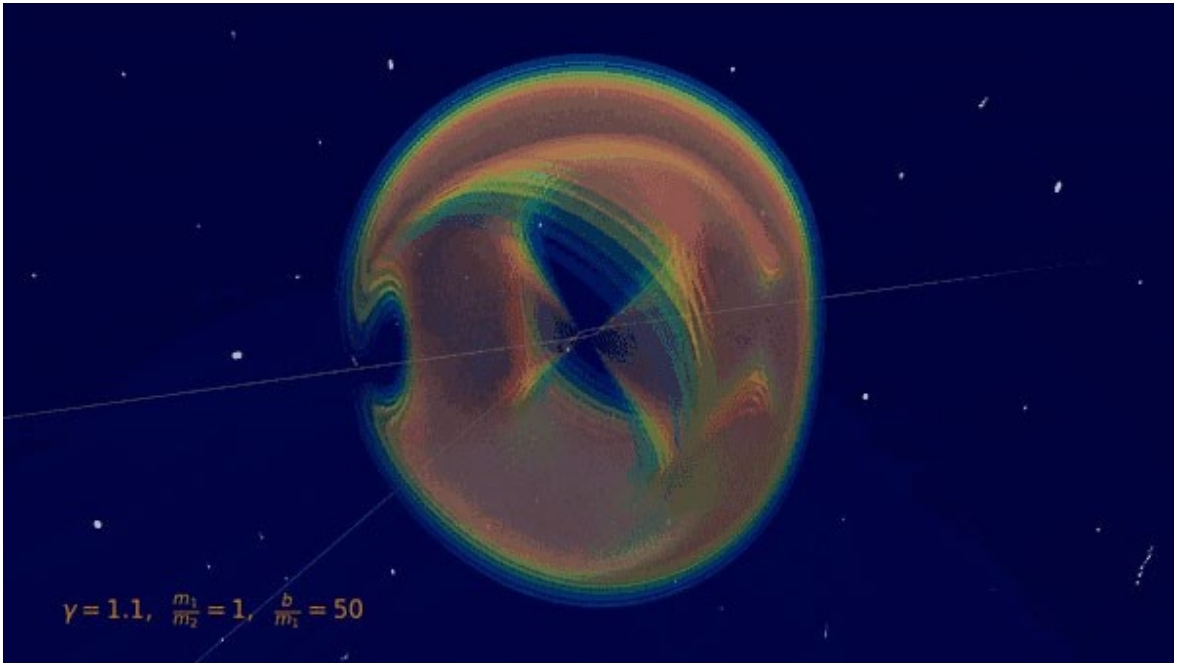
An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles

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. Bayrak 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. F. Montoya, J.-P. Correa-Baena, J. Qiu, J. Wang, K. Sveinbjörnsson, K. Hirselandt, 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. Saliba, M. Anaya, M. Veldhoen, N. Arora, O. Shargaieva, O. Maus, O. S. Game, O. Yudilevich, P. Fassl, 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, Y.-H. Chiang, Z. Iqbal, Z. Xie, and E. Unger

Nat Energy 7 (2022) 107

DOI: 10.1038/s41560-021-00941-3

Bremsstrahlung of black holes & neutron stars from quantum field theory



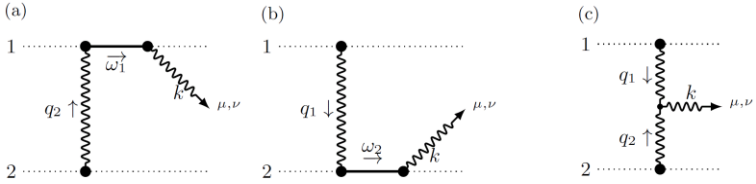
Visualization of the gravitational Bremsstrahlung from the scattering of two black holes (BSc thesis O. Babayemi)

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 Member Jan Plefka, a new approach to determining these waveforms (Fig. 1) and the deflections using methods of perturbative quantum field theory was 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 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 (Fig. 2). 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.



Feynman graphs to determine the waveform. The dotted lines represent the black holes, the waves represent gravitational radiation, and the lines represent fluctuations in the black hole's orbit.

SUSY in the sky with gravitons
G. U. Jakobsen, G. Mogull, J. Plefka, and J. Steinhoff
JHEP 2201 (2022) 027
arxiv: 2109.04465

2023

Highly efficient p-i-n perovskite solar cells that endure temperature variations
G. Li, Z. Su, L. Canil, D. Hughes, M. H. Aldamasy, J. Dagar, S. Trofimov, L. Wang, W. Zuo, J. J. Jerónimo-Rendon, M. M. Byranvand, C. Wang, R. Zhu, Z. Zhang, F. Yang, G. Nasti, B. Naydenov, W. C. Tsoi, Z. Li, X. Gao, Z. Wang, Y. Jia, E. Unger, M. Saliba, M. Li, and A. Abate
Science 379 (2023) 399
DOI: 10.1126/science.add7331

Interface engineering for high-performance, triple-halide perovskite–silicon tandem solar cells
S. Mariotti, E. Köhnen, F. Scheler, K. Sveinbjörnsson, L. Zimmermann, M. Piot, F. Yang, B. Li, J. Warby, A. Musiienko, D. Menzel, F. Lang, S. Keßler, I. Levine, D. Mantione, A. Al-Ashouri, M. S. Härtel, K. Xu, A. Cruz, J. Kurpiers, P. Wagner, H. Köbler, J. Li, A. Magomedov, D. Mecerreyes, E. Unger, A. Abate, M. Stolterfoht, B. Stannowski, R. Schlatmann, L. Korte, and S. Albrecht
Science 381 (2023) 63
DOI: 10.1126/science.adf5872

Device Performance of Emerging Photovoltaic Materials (Version 3)
O. Almora, D. Baran, G. C. Bazan, C. I. Cabrera, S. Erten-Ela, K. Forberich, F. Guo, J. Hauch, A. W. Y. Ho-Baillie, T. J. Jacobsson, R. A. J. Janssen, T. Kirchartz, N. Kopidakis, M. A. Loi, R. R. Lunt, X.

Mathew, M. D. McGehee, J. Min, D. B. Mitzi, M. K. Nazeeruddin, J. Nelson, A. F. Nogueira, U. W. Paetzold, B. P. Rand, U. Rau, H. J. Snaith, E. Unger, L. Vaillant-Roca, C. Yang, H.-L. Yip, and C. J. Brabec
Adv. Energy Mater. 13 (2023) 2203313
DOI: 10.1002/aenm.202203313

Marcel makes now even better electron microscopy with AI

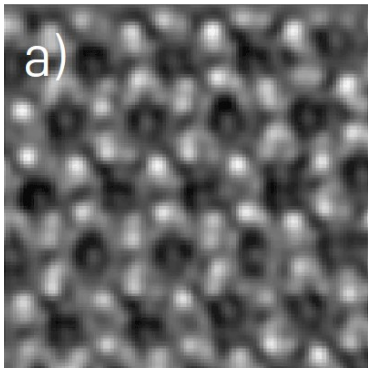
Our microscopes rank among the world's finest and highest-resolution instruments. With the NION HERMES microscope, we not only have the capability to visualize individual atoms but also to unveil their intrinsic properties. We can identify the type of atom, its bonding with neighbouring atoms, and characterize these neighbouring atoms, etc.

To perform these measurements, it is crucial to pinpoint the atomic positions efficiently, without excessive time or energy expenditure. Extended measurements risk atomic displacement, while excessive energy input can jeopardize our sample's integrity.

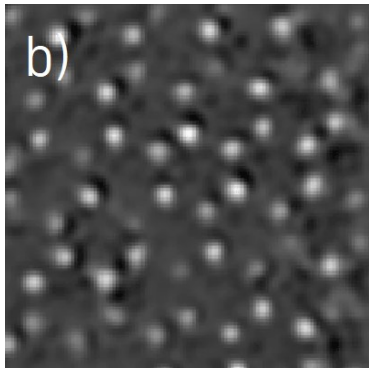
Marcel has implemented a clever strategy: He instructs his AI using previously acquired measurements to approximate the atoms' expected appearance. A handful of initial measurements

is now sufficient to gain an overview and predict the precise atom positions. This allows him to perform targeted measurements at these specific atomic locations."

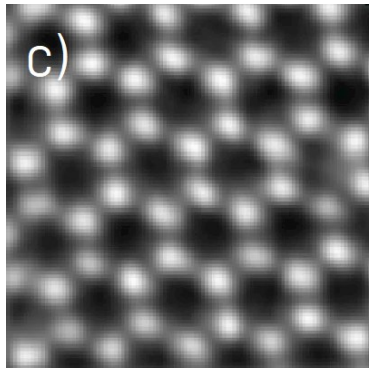
Ptychographic reconstructions of a MoS_2 (Molybdenum disulfide or just 'moly') sample with different scanning procedures:



a. Reconstruction from 250 random positions. The pattern is hardly visible.



b. Reconstruction from 250 AI-selected positions. You can see the hexagonal pattern and all single atoms.



c. Reconstruction from a slow conventional long grid scan (10000 positions)

If this technique could be integrated directly into the microscope's controller, it could actively search for the nearest point in real-time.

M. Schloz, J. Müller, T.C. Pekin *et al*.
Deep reinforcement learning for data-driven adaptive scanning in ptychography.
Sci. Rep. 13, 8732 (2023).
DOI: 10.1038/s41598-023-35740-1 or arXiv: 2203.15413

2024

Ion-induced field screening as a dominant factor in perovskite solar cell operational stability
J. Thiesbrummel, S. Shah, E. Gutierrez-Partida, F. Zu, F. Peña-Camargo, S. Zeiske, J. Diekmann, F. Ye, K. P. Peters, K. O. Brinkmann, P. Caprioglio, A. Dasgupta, S. Seo, F. A. Adeleye, J. Warby, Q. Jeangros, F. Lang, S. Zhang, S. Albrecht, T. Riedl, A. Armin, D. Neher, N. Koch, Y. Wu, V. M. Le Corre, H. Snaith, and M. Stolterfoht
Nat. Energy 9 (2024) 664
DOI: 10.1038/s41560-024-01487-w

Spinel-Structured High-Entropy Oxide Nanofibers as Electrocatalysts for Oxygen Evolution in Alkaline Solution: Effect of Metal Combination and Calcination Temperature
C. Triolo, K. Moulaee, A. Ponti, G. Pagot, V. Di Noto, N. Pinna, G. Neri, and S. Santangelo
Adv. Funct. Mater. 34 (2024) 2306375
DOI: 10.1002/adfm.202306375

Electrochemical Realization of 3D Interconnected MoS_3/PPy Nanowire Frameworks as Sulfur-Equivalent Cathode Materials for Li-S Batteries
H. Yu, A. Siebert, S. Mei, R. Garcia-Diez, R. Félix, T. Quan, Y. Xu, J. Frisch, R. G. Wilks, M. Bär, C. Pei, and Y. Lu
Energy Environ. Mater. 7 (2024) e12539
DOI: 10.1002/eem2.12539

A novel approach to the synthesis of amorphous metal-organic frameworks and coordination polymers

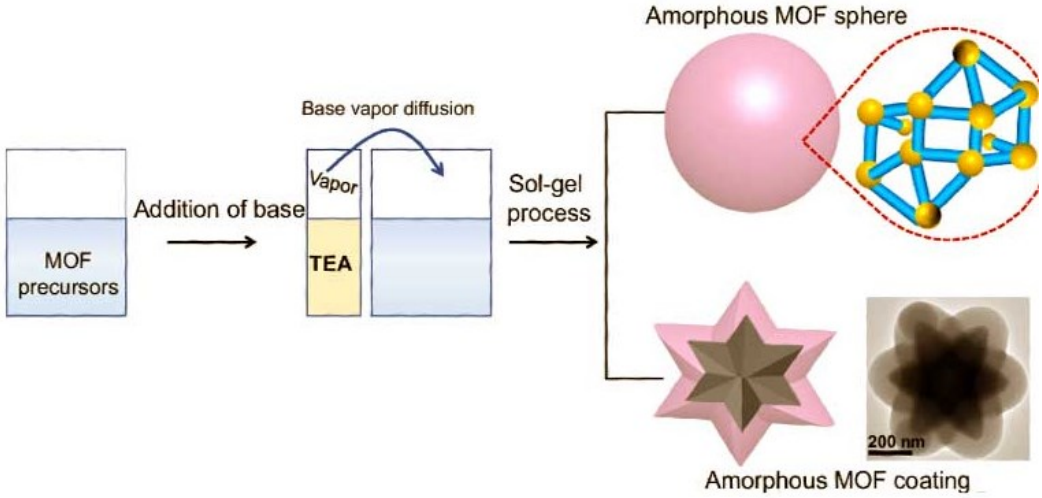
A team of researchers at Humboldt-Universität zu Berlin, led by IRIS Member Nicola Pinna, has made a significant breakthrough in the field of nanotechnology. The team has successfully extended the well-known Stöber method, originally used for amorphous SiO_2 colloids, to synthesise amorphous metal-organic frameworks (MOFs) and coordination polymers (CPs). Their innovative approach employs the slow, continuous diffusion of triethylamine (TEA) vapour to control the deprotonation of organic ligands with great precision, thereby enabling the creation of finely crafted amorphous CP spheres. This innovative approach is set to markedly enhance the functionality and complexity of colloidal materials, thereby paving the way for new applications in technology and medicine.

The synthesis of amorphous MOFs and CPs is initiated by the introduction of triethylamine (TEA) vapor to a solution comprising metal ions and organic ligands. This initiates the deprotonation process, allowing the ligands to bond with the metal ions and form intricate amorphous MOF or CP structures. The versatility of this method has been demonstrated by the successful synthesis of 24 distinct amorphous CP spheres, created by selecting 12 metal ions and 17 organic ligands.

Furthermore, the introduction of functional nanoparticles has enabled the synthesis of uniform core-shell colloids with conformal amorphous CP coatings.

The method's gradual deprotonation process enables the heterogeneous nucleation of amorphous MOFs on any substrate, irrespective of its chemical composition, structure, or morphology. This adaptability has facilitated the synthesis of over 100 core-shell colloids, combining 20 different amorphous MOF or CP shells with more than 30 different core-nanoparticles, each with distinct properties and potential applications. Furthermore, these core-amorphous MOF shell colloids can readily be transformed into a variety of functional colloids through the application of liquid-phase or solid-state processes.

It is particularly encouraging to note that these amorphous-based core-shell colloids have the potential to serve as sacrificial templates for the creation of multifunctional nanostructures. Yolk-shell structures, which resemble core-shell structures but feature voids between the core and shell, are particularly promising for use in catalytic reactions, energy storage solutions and advanced drug delivery systems. This advancement marks a significant step forward in nanotechnology, offering researchers a robust tool for the systematic design of advanced colloidal materials exhibiting different levels of functionality and complexity, and thus expanding the horizons of material science.



The synthesis of aMOFs and aCPs colloids and core-shell structures via mimicking the Stöber method.

Stöber method to amorphous metal-organic frameworks and coordination polymers
W. Zhang, Y. Liu, H.S. Jeppesen, and N. Pinna
Nat. Commun. 15, 5463 (2024).
DOI: 10.1038/s41467-024-49772-2

7. The Legacy of IRIS Adlershof

While IRIS Adlershof is concluding, its legacy will endure through the ongoing projects *Kolleg Mathematik Physik Berlin (KMPB)* and *Center for the Science of Materials Berlin (CSMB)*.

Kolleg Mathematik Physik Berlin

In the Berlin area, a strong scientific interest in interdisciplinary research between mathematics and physics has flourished, particularly with the establishment of the bridging professorships of Matthias Staudacher in 2010 and Alexander von Humboldt Professor Dirk Kreimer in 2011. These two appointments have given the CRC 647 Space-Time-Matter, which has already been running since 2005 under the spokesmanship of IRIS Member Jochen Brüning, a strong impetus for further successful work. In the last funding period, Matthias Staudacher took over as spokesperson. Together, these developments focused on the mathematical structures and foundations of quantum field theory and quantum gravity, especially their connections to arithmetic and algebraic geometry. In 2016 this collaboration culminated in the founding of an interdisciplinary center at Humboldt-Universität zu Berlin, the *Kolleg Mathematik Physik Berlin*.

KMPB is jointly led by Matthias Staudacher and Nichol Furey, both members of IRIS Adlershof.

Center for the Science of Materials Berlin

By establishing the *Center for the Science of Materials Berlin (CSMB)* in 2022, Humboldt-Universität zu Berlin committed to develop solutions for key global challenges related to future energy supply and sustainable use of resources, as well as communication, safety, and health. Many, if not all, of these seemingly disconnected areas have one common ground: They rely on materials with properties tailored to their respective tasks. Yet, materials used today have either already reached their performance limits or soon will. In order to master the pressing challenges related to minimize energy demands and to close material cycles, it is essential to identify and evaluate novel materials and material systems, and to develop them to relevant technological maturity.

The CSMB is headed by Stefan Hecht and his deputy Emil List-Kratochvil, both members of IRIS Adlershof.

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