Integrative Research Institute for the Sciences

Annual Report 2013 & 2014

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Foreword

The *Integrative Research Institute for the Sciences* **IRIS Adlershof** was founded in June 2009 upon the initiative of nine scientists from Humboldt-Universität’s departments of chemistry, computer sciences, mathematics and physics. It is the prototype of an innovative research format of the Humboldt-Universität zu Berlin - the *Integrative Research Institute (IRI)* that was developed within the framework of the university’s future concept for the Excellence Initiative of the German federal and state governments. Its goal is to provide outstanding scientists with excellent infrastructure for interdisciplinary research in the sciences. **IRIS Adlershof** builds on the special competences of Humboldt-Universität at its Campus Adlershof in the fields of Modern Optics, Molecular Systems, Mathematical Physics, and Computation in the Sciences. A particular goal for **IRIS Adlershof** is to establish itself as an international leader in the research areas "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter"

Since its inception, **IRIS Adlershof** has developed remarkably. Two years ago, we reported on the activities during our start-up phase from 2009 to 2012. The present report reflects the years 2013 and 2014. It includes important national and european research projects, such as collaborative research centers, research training groups, and EU initial training networks, which have been successfully established. Particularly important for the long run, we have managed to raise federal and state funds for the construction of a research building for the IRIS research area "Hybrid Systems for Optics and Electronics".

Many thanks to all the members and the staff of **IRIS Adlershof**, without whose dedicated work this report would have remained empty. We are also very grateful for the wide range of support that we have received from the administrative departments and the President’s office of Humboldt-Universität zu Berlin.

Best wishes,

Jürgen P. Rabe

Founding Chairman

Contents

1 The Integrative Research Institute for the Sciences

The development plans of *Humboldt-Universität zu Berlin (HU)* for research strategies are based on a sustainable intensification of its scientific profile and on networking with strategic national and international partners with the clear goal to create key concentrations in research areas that show the HU's excellent strengths and give it an outstanding international presence. This goal can only be successfully achieved by recognizing to a certain degree that many fundamental scientific problems are difficult to solve, if only seen from the sole perspective of the individual scientific disciplines. Therefore, within the framework of its federally and nationally funded Excellence Initiative, the HU has set up Integrative Research Institutes (IRIs) that enable and promote top research by bridging the different disciplines. The aim of these innovative structures is to connect the HU's existing core competences with outside research and industry partners in order to create an efficient structure for seminal interdisciplinary cooperation plans as well as to further the development of early-stage scientists. The HU is thus responding to the so-called pillarization of the German higher education and science system that is still making it hard to optimally access the existing research potential from the interface of university and non-university research institutes.

The first IRI that the HU founded was the Integrative Research Institute for the Sciences **IRIS Adlershof**, which was established on its natural science campus at Berlin-Brandenburg's top science, business, and media hub Berlin-Adlershof in summer 2009. This IRI interdisciplinarily 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 bridge professors for 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 the Humboldt-Universität with pertinent non-university institutes and innovative enterprises. **IRIS Adlershof** has dedicated itself to two research areas: "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter".

1.1 Members of IRIS Adlershof

IRIS Adlershof was founded in July 2009 upon an initiative of nine researchers from the Humboldt-Universität zu Berlin and currently consists of 17 members.

With great dismay and sadness, we have to report that our highly valued founding member and colleague, Professor Fritz Henneberger, died suddenly and completely unexpectedly in the beginning of 2015. Professor Henneberger was a scientist with a very high international reputation in the field of modern optics and photonics. Especially as spokesman for Collaborative Research Centre 951, one of our most important and prestigious projects, he made a major contribution to the successful development of **IRIS Adlershof**. We will never forget him.

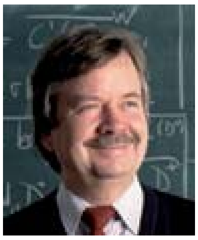
During the reporting period Christian Limberg, Professor for Inorganic and General Chemistry at the Humboldt-Universität zu Berlin, was elected as a new IRIS-member.

IRIS members are typically also members of a scientific department from the Humboldt-Universität and/or of non-university research institutes.

Members

Ballauff, Matthias, Prof. Dr.
Helmholtz-Zentrum Berlin für Materialien und Energie and
Humboldt-Universität zu Berlin, Department of Physics
Research Area: Soft Matters and Funcional Materials

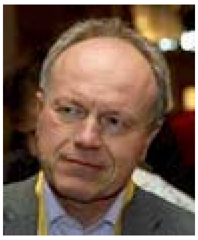
Benson, Oliver, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Physics
Research Area: Nano Optics



Brüning, Jochen, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Mathematics
Research Area: Geometric Analysis and Spectral Theory

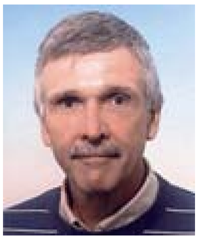
Draxl, Claudia, Prof. Dr. *(Einstein Professorship)*
Humboldt-Universität zu Berlin, Department of Physics and
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Research Area: Theoretical Solid State Physics

Elsässer, Thomas, Prof. Dr.
Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy and
Humboldt-Universität zu Berlin, Department of Physics
Research Area: Nonlinear Optics and Short Pulse Spectroscopy



Freytag, Johann-Christoph, Prof. Ph.D.
Humboldt-Universität zu Berlin, Department of Computer Science
Research Area: Databases and Information Systems

Hecht, Stefan, Prof. Ph.D.
Humboldt-Universität zu Berlin, Department of Chemistry
Research Area: Organic Chemistry and Functional Materials



Henneberger, Fritz, Prof. Dr. († 2015)
Humboldt-Universität zu Berlin, Department of Physics
Research Area: Photonics

von Klitzing, Regine, Prof. Dr.
Technische Universität Berlin, Department of Chemistry
Research Area: Applied Physical Chemistry

Koch, Norbert, Prof. Dr. *(Deputy Chairman of IRIS Adlershof)*
Bridging Professorship Physics/Chemistry
Humboldt-Universität zu Berlin, Department of Physics and
Helmholtz-Zentrum Berlin für Materialien und Energie
Research Area: Supramolecular Systems

Kramer, Jürg, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Mathematics
Research Area: Arithmetic Geometry, Math Education

Kreimer, Dirk, Prof. Dr. *(Alexander von Humboldt Professorship)*
Humboldt-Universität zu Berlin
Department of Mathematics and Department of Physics
Research Area: Structure of Local Quantum Field Theories

Limberg, Christian, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Chemistry
Research Area: Coordination Chemistry & Catalysis

Plefka, Jan, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Physics
Research Area: Quantum Field and String Theory

Rabe, Jürgen P., Prof. Dr. *(Founding Chairman of IRIS Adlershof)*
Humboldt-Universität zu Berlin, Department of Physics and
Max Planck Institute for Colloids and Interfaces
Research Area: Physics of Macromolecules

Reinefeld, Alexander, Prof. Dr.
Zuse Institute Berlin and
Humboldt-Universität zu Berlin, Department of Computer Science
Research Area: Parallel and Distributed Systems

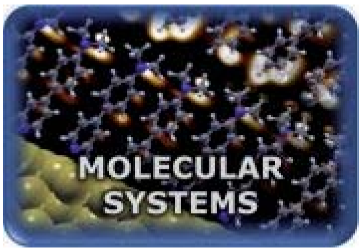
Sauer, Joachim, Prof. Dr.
Humboldt-Universität zu Berlin, Department of Chemistry and
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Research Area: Quantum Chemistry

Staudacher, Matthias, Prof. Dr. *(Board Member of IRIS Adlershof)*
Bridging Professorship Physics/Mathematics
Humboldt-Universität zu Berlin,
Department of Mathematics and Department of Physics
Research Area: Mathematical Physics of Space, Time and Matter

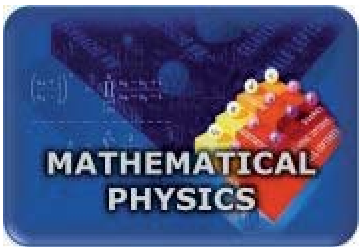
1.2 Competences of IRIS Adlershof

IRIS Adlershof builds on the special competences of Humboldt-Universität in the fields of modern optics, molecular systems, mathematical physics, and computation in the sciences.

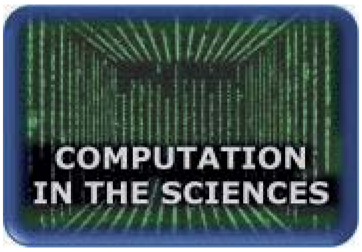
In the competence field **Modern Optics,** the unique properties of light with very precisely defined time and wavelength structures in a broad spectral range are employed to forge ahead in currently inaccessible terrains in physics by using a combination of modern optical methods. Fundamental processes in nature or in artificial materials will thus be elucidated, and this insight will be employed for novel applications for optical technologies, modern information processing and storage, sensors, material processing, and medicine.



In the competence field of **Molecular Systems,** the interaction of structural, electronic, optical, and chemical properties is investigated at different levels of complexity. Inspired by a fundamental understanding of the relationship between structure and physico-chemical function in natural systems, new approaches to artificial systems with unprecedented property profiles are being developed that shall finally lead to new types of energy and resource saving materials and functional systems.



Mathematical Physics investigates the geometry and analysis of mathematical structures at the interface between theoretical physics and pure mathematics, as discussed, e.g., in superstring theories and quantum field theories. With the new Large Hadron Collider (LHC) at CERN, particle physics is at the onset of a new era, which makes this topical field very timely. A related but differently oriented research field is "Complex Dynamics" which currently finds its most interesting applications in climate research and in the physics of biomacromolecules.



Computation in the Sciences is dedicated to the computer simulation of real systems that can be analyzed with scientific methodologies. It supplements the traditional approaches in science and mathematics, which are based on collecting empirical evidence, on the one hand, and conceptual and algorithmic modeling on the other. With the rapid development of the architecture of high performance computing, new dimensions for the extraction of quantitative information will be within reach. Additionally, more and more realistic images of reality can be created by using efficient algorithms.

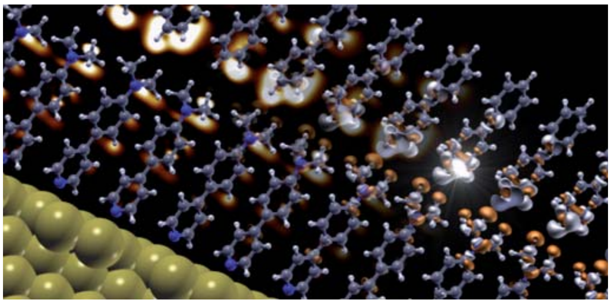
Each of these competence fields encourages close cooperation across the disciplinary boundaries of physics, chemistry, mathematics, and computer sciences. The interdisciplinary nature of **IRIS Adlershof** has been further strengthened by filling "Bridge Professorships" between mathematics and physics, "Mathematical Physics of Space, Time, and Matter", and between physics and chemistry, "Supramolecular Systems".

1.3 Research Areas

IRIS Adlershof is currently devoted to two prime areas of research: "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter".

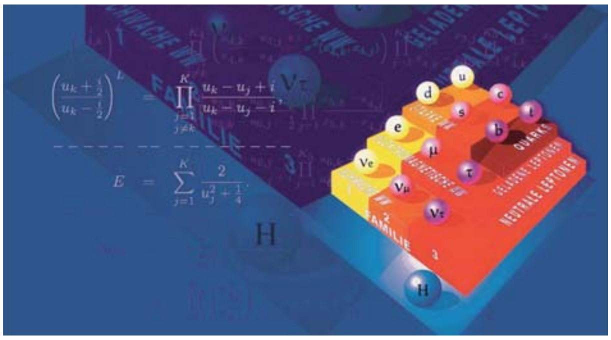
1.3.1 Hybrid Systems for Optics and Electronics

Hybrid inorganic/organic systems structured on atomic, molecular and mesoscopic length scales offer completely new possibilities 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 will be investigated and explored for their application potential.



1.3.2 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. Therefore, it is necessary to analyze the role of basic symmetries as well as the way they are broken. The ultimate goal is to find the "Weltformel", in order to describe the fundamental forces and their interactions by a single coherent theory. Hopefully it will become clear along the way how the "smooth" world that we experience emerges from the "chaotic" principles of quantum physics. Mathematicians and theoretical physicists are cooperating to address specific questions of mathematical physics in the described framework. An important structural goal consists in broadening the base of this enterprise by also including fundamental experimental physics.



2 Development of IRIS Adlershof during the Reporting Period

In 2013 and 2014, the time period covered by this report, the research at **IRIS Adlershof** focused on its two main research areas: "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter".

Highlights within the first named research area are the Collaborative Research Center (CRC) 951 "Hybrid Inorganic/Organic Systems for Opto-electronics" (HIOS), the CRC 1109 "Understanding of Metal Oxide/Water Systems at the Molecular Scale: Structural Evolution, Interfaces, and Dissolution", and the Helmholtz Energy Alliance "The Best of Two Worlds: Inorganic/Organic Hybrid Building Elements and Techniques for Photovoltaics and Solar Fuel Production". Further coordinated joint projects were funded by various federal, state, and international funding institutions (see Chapter 3).

Most important for the future development of this research area is the successful securing of funds for a new research building for "Hybrid Systems for Electronics, Optoelectronics and Photonics" with the German Science Council (Wissenschaftsrat). With its decision the Science Council evaluated **IRIS Adlershof**'s research approach as highly significant for the country. The combination of organic and inorganic materials is attested uniqueness complementary to programs at other German research centers.

The second named IRIS research area "Space-Time-Matter" has likewise developed very well. This is reflected by the approvals of further funding periods for the CRC 647 "Space-Time-Matter: Analytic and Geometric Structures" as well as for the Research Training Group (RTG) 1504: "Mass, Spectrum, Symmetry: Particle Physics in the Era of the Large Hadron Collider". Furthermore, a new project "Gravitation and High Energy Physics" has been funded by the Einstein Foundation.

Annually more than 100 invited lectures and articles in peer-reviewed scientific journals each, as well as a number of patents, reflect the high research output in **IRIS Adlershof**'s main research areas. Several honors, including Prof. Claudia Draxl's appointment as a Max-Planck-Fellow, Prof. Jürg Kramer's election as a member of the National Academy of Science and Engineering (acatec), and Prof. Jochen Brüning's election as a member of the Institute for Advanced Study in Princeton with a corresponding research stay there during the academic year 2012/13, have further increased IRIS's visibility.

In total, the IRIS members have obtained extensive third-party funding in the report period. The amount managed by the Humboldt-Universität comes to 16 million euros. The existing as well as new research cooperations with partner institutions have been further developed. For instance, a KOSMOS Summer University with the topic "Chemistry and Physics of Novel Materials" jointly held with Princeton University and the National University of Singapore, took place at the Adlershof campus in July 2014. Further examples include a cooperative project that started in 2013 between **IRIS Adlershof**, the IRI for the Life Sciences, and Tel Aviv University on "Biological and Soft-Matter Physics", and a collaboration with the Fraunhofer Institute for Applied Polymer Research.

IRIS Adlershof's start-up and interim funding allowed to support a number of excellent early-stage researchers in both IRIS's focal research areas. Together with Helmholtz-

Zentrum Berlin (HZB) a graduate school was set up on the topic "Hybrid Materials for Efficient Energy Generation and Information Technologies" (Hybrid4Energy).

In summary, **IRIS Adlershof**'s international visibility has considerably improved and the Adlershof Campus has continued to make a name for itself as a top research site during the report period.

2.1 Infrastructure and Finance

2.1.1 Spatial Infrastructure

An important part of our efforts was to extend the **IRIS Adlershof**'s infrastructure. In the early stages of its founding, which were completed in October 2012, **IRIS Adlershof** was decentrally located because of the lack of suitable rooms. The condensation nucleus for the required spatial merger of IRIS research groups was the completion, just before the beginning of the report period, of the first construction phase at Zum Großen Windkanal 6, which was a former barracks and now site of the IRIS building. The IRIS administration and research groups of Prof. Draxl and Prof. Staudacher were the first ones to move into the section of the building that was top renovated and funded by the University. The building's modern, well-equipped conference rooms, lecture halls, and commons rooms have had a quite positive influence on the integrative research cooperations and led to synergies. In addition to the work groups, the graduate school SALSA and CRC 951, whose main offices are in the IRIS building, have also profited from being there. The building from the second phase of construction that was completed in the second quarter of 2014 was also turned over to IRIS. The Plefka group, the Humboldt-ProMINT-Kolleg, which is connected to IRIS because of its content, parts of CRC 951, and the main office for the new CRC 1109 "Understanding of Metal Oxide/Water Systems at the Molecular Scale: Structural Evolution, Interfaces, and Dissolution" could move in.

When the IRIS building was completely finished, the conditions noticeably improved for the IRIS groups doing theoretical work. The structural conditions, however, did not allow highly specialized laboratories to be implemented in the same building. As a result, the IRIS groups that do experiments have had to use decentralized laboratories at their respective departmental institutes. For successful work in the research area "Hybrid Systems for Optics and Electronics", the still largely separated worlds of chemistry and physics needed to be integrated in the form of a joint research project, which put very specific demands on both the participating scientists as well as the infrastructure they would use.

It was also essential for the project's success that the experimenters, who came from chemistry, physics, and materials science, were able to set up in the same research building not only with meeting areas but also first-rate laboratories that were especially equipped for interdisciplinary work. An application for funding of a research building for IRIS was submitted in January 2013 regarding an Article 91b GG procedure.

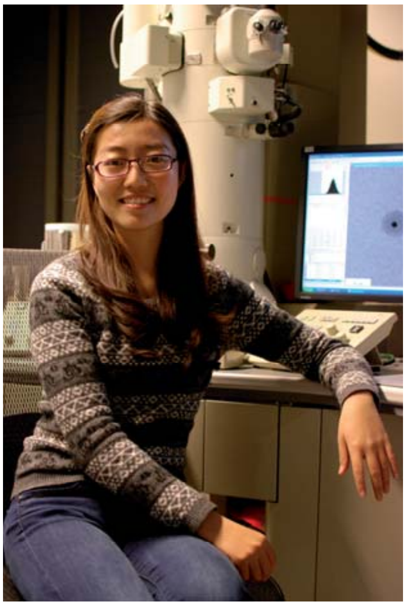
Visualization: Nickl & Partner Architekten AG

A main element in the application for the research building was a group lab with standardized clean and grey room conditions. The Science Council recommended this application for support, which proves the international importance of this research topic. The Joint Science Council of the federal and state governments followed this recommendation and approved the research building application in June 2013. The federal and state governments have allocated a total of 44 million euros to finance this building project. The project supervisor, which is the Senate Department for Urban Development and the Environment, has chosen a conceptual preliminary draft that will now be realized. The Nickl & Partner architects and the IDK Kleinjohann planning office developed a concept that visualized an independent, striking building structure, which naturally fits in with the existing IRIS buildings and integrates a further former barrack, thereby presenting **IRIS Adlershof** as a cohesive research institution. The new building will be placed as the connecting piece between the two existing buildings. This way, there will still be a representational exterior courtyard-like space facing the street, Zum Großen Windkanal, that will function together with the foyer as a common entrance area and bridging element between the various **IRIS Adlershof** research groups. The construction work will start in the spring of 2016 and the finished building complex should be ready for moving in and working in by the end of 2018.

2.1.2 Core Facilities of IRIS Adlershof

For structural analysis at Adlershof, the **Joint Laboratory for Structural Research (JLSR)** was established as a joint institution of the HU, the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) and the Technische Universität Berlin (TU Berlin) under the roof of **IRIS Adlershof**.

The JLSR provides and develops infrastructure for structural research on organic, inorganic, and the corresponding hybrid materials and systems. It focuses on microscopy, scattering, and lithography using electrons, x-rays, and scanning probes.



The laboratory combines different structural research methods that had been separated before at either the HU or the HZB. It spans a field of work that ranges from crystalline semiconductor and insulator materials via organic molecular and supramolecular systems to biomaterials. An essential feature of this research is a non-destructive analysis of the local structure as possible from the atomistic length range up to macroscopic dimensions of objects with all the currently available methods. A cryogenic transmission electron microscope was purchased for a non-destructive analysis of samples from the fields of soft matter and biological sciences. At the end of the reporting period, the JLSR infrastructure was completed by purchasing a TERS (Tip-Enhanced Raman-Spectroscopy) microscope.

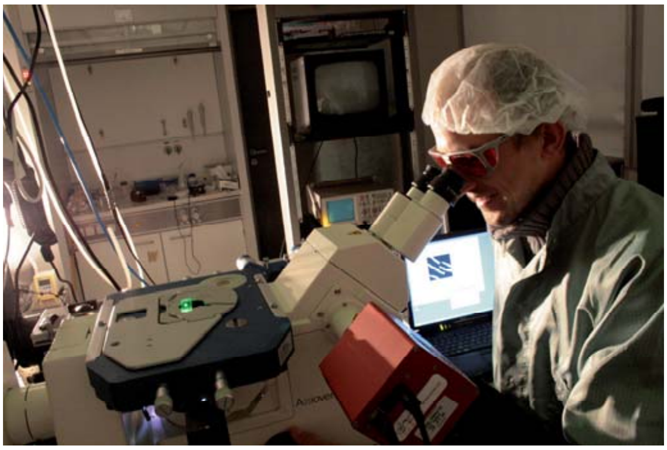
The JLSR is a facility of **IRIS Adlershof**, in which the HU cooperates with the HZB and the TU Berlin. We were able to obtain more cooperation partners from the Ferdinand-Braun-Institut, the Max-Born-Institut, the Paul-Drude-Institut, the Fraunhofer Institute for Applied Polymer Research, the Leibniz Institute for Crystal Growth (IKZ), and the Federal Institute for Materials Research and Testing (BAM).

Participating IRIS members:

- Prof. Dr. Matthias Ballauff
- Prof. Dr. Regine von Klitzing
- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

The OPen Access Laboratory (OPAL) is a new concept for the promotion of collaboration between **IRIS Adlershof** and pertinent scientific and industrial partners. Innovative high-tech enterprises and research institutes have been invited to collaborate within OPAL by sending their own personnel. The OPAL for Advanced Materials’ goal is to develop and implement tailored concepts for organic and molecular electronics.

Two other OPALs for analytical science and for modern optics are currently under construction.



Another goal is to obtain knowledge that can be efficiently transferred in research to interested companies to support the fastest possible implementation of new competitive products.

Participating IRIS members:

- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

Industrial cooperation partners:

- Atotech Deutschland GmbH
- JPK Instruments
- Novaled GmbH
- PlasmaChem GmbH

2.1.3 Finances

In the report period, **IRIS Adlershof** annually received a basic financial support of 200,000 euros to cover its main office costs from the University's central funding.

In the second round of the Excellence Initiative of the federal and state governments, **IRIS Adlershof** was involved in all three funding areas and was therefore able to contribute to the successful acquisition of graduate schools and clusters of excellence and to its future concept. In addition, **IRIS Adlershof** has successfully applied for funding of up to 60 million euros in the reporting period. Most of this amount was attributable to the IRIS Research Building (44 million euros). A further 16 million euros was raised for externally/ third party funded research projects.

2.2 Cooperations

IRIS Adlershof lives through its academic members, who are primarily university professors but are also linked in many different ways with their partners outside the university. For example, joint professorships (also known as special professorships) establish a firm link between university and non-university research facilities and play a very important role in the constant exchange of knowledge. The Humboldt-Universität appoints special professors to full professorships but these individuals must also fulfill a leadership role in a non-university research facility. Therefore **IRIS Adlershof** is linked to extra-faculty partner institutions as well.

IRIS Adlershof sees itself, among other things, as a platform for the development of scientific cooperation with strategic partners on site at Adlershof, in the Berlin-Brandenburg region, and beyond. The extension and establishment of existing and new research cooperations are rated very highly. The intensive collaboration with HU's first two profile partners, Princeton University and National University of Singapore, on "Novel (Opto-) Electronic Materials" is therefore particularly important.

In October 2013, the first joint workshop with Princeton University took place at Berlin Adlershof, which discussed ways and opportunities to work on concrete joint research projects as well as to set up a steady exchange of scientists and students. This was followed up by a second workshop in March 2014 in Princeton. An application for a DFG and NSF financed international research training group is in preparation. A twelve-day KOSMOS Summer School on "Chemistry and Physics of Novel Materials for (Opto-)Electronics" was held with Princeton University and the National University of Singapore.

Jürgen P. Rabe, Professor at the Department of Physics and Chairman of **IRIS Adlershof**, was appointed visiting professor at the Department of Chemistry at Princeton University during Spring Term 2014. He worked together with Professor Steven L. Bernasek on organic-inorganic hybrid systems, and he taught a graduate course for graduate students in physics and chemistry, and at the School of Engineering and Applied Sciences.

Together with the IRI for the Life Science and Tel Aviv University, a cooperation project on "Biological and Soft Matter Physics" began as well, which was initially planned for three years and has also originated in a workshop in Berlin. In a second step, at the beginning of 2014, concrete project proposals were chosen for implementation. A basic element of the program was to exchange scientists and students.

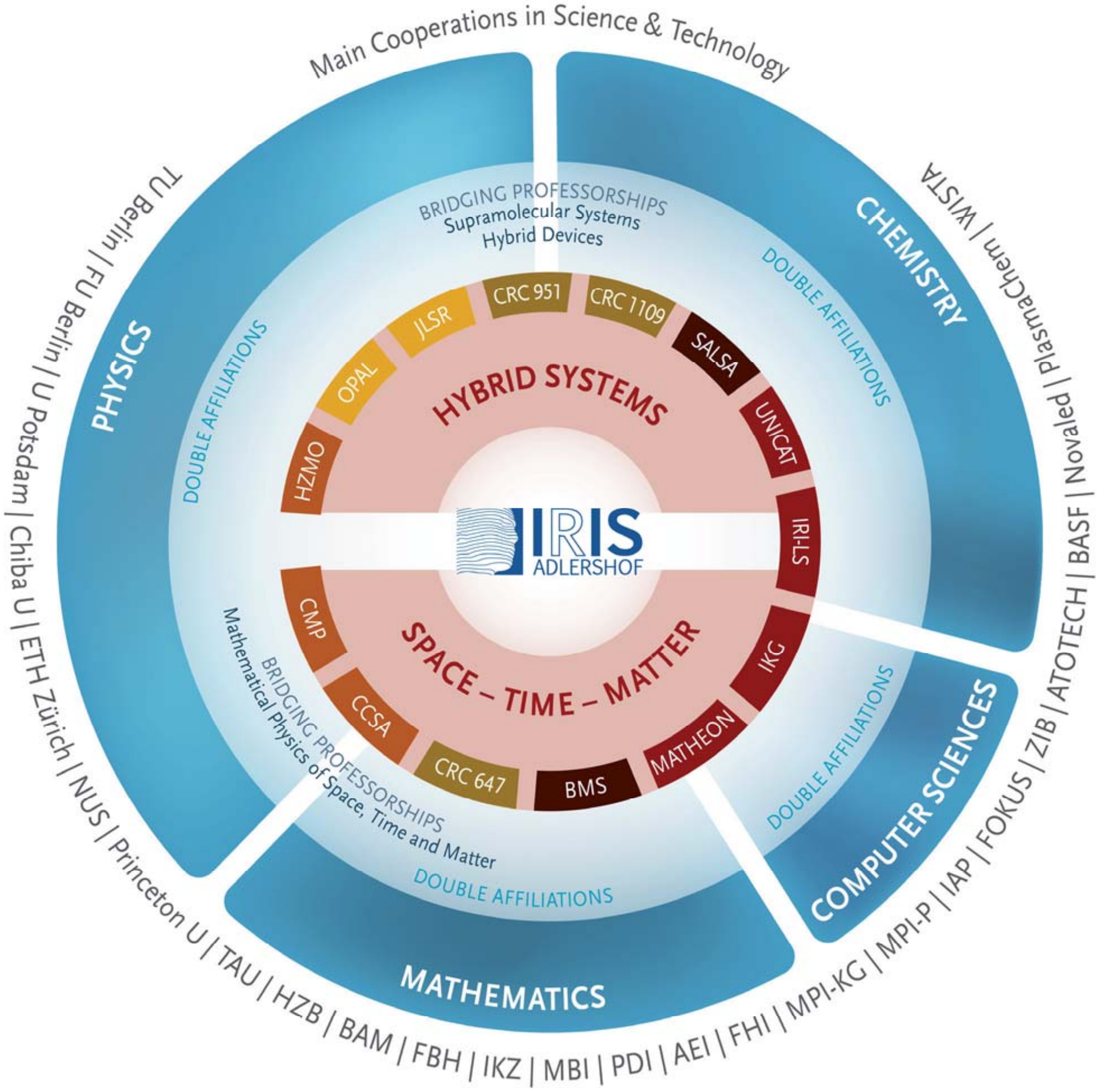
Cooperations for the Open Access Laboratory (OPAL) for Advanced Materials were noticeably intensified in 2013 by extending the joint research program with Atotech Deutschland GmbH to include thermoelectric materials for energy production. OPAL even started collaboration with Novaled GmbH, a leading worldwide company for displays and LEDs based on organic materials, which led to a cooperation contract in 2015. The Fraunhofer Institute for Applied Polymer Research (IAP), Potsdam-Golm, could be gained as a strategic partner for the development of production processes from hybrid components. The completion of the corresponding cooperation contract required a basic agreement between the HU and the Fraunhofer Society, which was worked out in the report period and is now being voted on.

Professor Norbert Koch, a member of **IRIS Adlershof**, was appointed Chair Professor of the Functional Nano & Soft Materials Laboratory (*FUNSOM*), a key institute of Soochow University in Suzhou, China. Moreover, he has been appointed as Visiting Professor at Chiba University, Japan. **IRIS Adlershof** is cooperating, in particular, with the group of Professor Nobuo Ueno and with the *Graduate School of Advanced Integration Science* of Chiba University.

Through the approval of the Einstein program projects "Gravitation and High Energy Physics" and "Active Plasmonic Nano-Antennas for Generation, Detecting, and Converting Quantum Light", the two existing scientific collaborations with the MPI for Gravitation Physics Potsdam (Albert-Einstein Institute) could be strengthened and a new cooperation with Hebrew University Jerusalem begun.

Professor Jan Plefka spent a sabbatical semester at the renowned Institute for Theoretical Physics at ETH Zürich. He researched the topic of mathematical physics together with the Zürich colleagues. This exchange has strengthened **IRIS Adlershof**’s cooperation with ETH.

The following graphic shows the most important cooperation partners of **IRIS Adlershof:**



AEI	Max Planck Institute for Gravitational Physics (Albert Einstein Institute) (Max-Planck-Institut für Gravitationsphysik (Albert-Einstein-Institut))
ATOTECH	Atotech Deutschland GmbH
BAM	Federal Institute for Materials Research and Testing (Bundesanstalt für Materialforschung und –prüfung)
BASF	BASF - The Chemical Company
BMS	Berlin Mathematical School
CCSA	Center of Computational Sciences Adlershof
Chiba U	Chiba University - Graduate School of Advanced Integration Science
CMP	Center for Mathematical Physics (planned)
CRC 647	Collaborative Research Center 647 Space-Time-Matter. Analytic and Geometric Structures (Sonderforschungsbereich 647 "Raum-Zeit-Materie. Analytische und Geometrische Strukturen")

CRC 951	Collaborative Research Center 951 Hybrid Inorganic/Organic Systems for Opto-Electronics
CRC 1109	Collaborative Research Center 1109 Understanding of Metal Oxide/Water Systems at the Molecular Scale: Structural Evolution, Interfaces, and Dissolution
ETH Zürich	Eidgenössische Technische Hochschule Zürich
FBH	Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik
FHI	Fritz-Haber-Institut der Max-Planck-Gesellschaft
FOKUS	Fraunhofer Institute for Open Communication Systems (Fraunhofer-Institut für Offene Kommunikationssysteme)
FU Berlin	Freie Universität Berlin
HZB	Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
HZMO	Humboldt Center for Modern Optics (Humboldt Zentrum für Moderne Optik)
IAP	Fraunhofer Institute for Applied Polymer Research (Fraunhofer-Institut für Angewandte Polymerforschung)
IKG	Image Knowledge Gestaltung. An Interdisciplinary Laboratory (Bild Wissen Gestaltung. Ein interdisziplinäres Labor)
IKZ	Leibniz Institute for Crystal Growth (Leibniz Institut für Kristallzüchtung)
IRI-LS	Integrative Research Institute (IRI) for the Life Sciences
JLSR	Joint Laboratory for Structural Research
MATHEON	DFG Research Center MATHEON (DFG-Forschungszentrum MATHEON)
MBI	Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie)
MPI-KG	Max Planck Institute of Colloids and Interfaces (Max-Planck-Institut für Kolloid- und Grenzflächenforschung)
MPI-P	Max Planck Institute for Polymer Research (Max-Planck-Institut für Polymerforschung)
Novaled	Novaled GmbH
NUS	National University of Singapore
OPAL	OPen Access Laboratory
PDI	Paul-Drude-Institut für Festkörperelektronik
PlasmaChem	PlasmaChem GmbH
Princeton U	Princeton University
SALSA	School of Analytical Sciences Adlershof
TAU	Tel Aviv University
TU Berlin	Technische Universität Berlin
UNICAT	Cluster of Excellence "Unifying Concepts in Catalysis"
U Potsdam	University of Potsdam (Universität Potsdam)
WISTA	WISTA Management GmbH
ZIB	Zuse Institute Berlin (Konrad-Zuse-Zentrum für Informationstechnik Berlin)

3 Coordinated Collaborative Projects with Participating IRIS Members

3.1 IRIS Adlershof in the Excellence Initiative

IRIS Adlershof members are involved in the clusters of excellence: "Image Knowledge Gestaltung. An Interdisciplinary Laboratory" and "Unifying Concepts in Catalysis – UniCat" as well as in the School of Analytical Sciences Adlershof (SALSA) and the Berlin Mathematical School (BMS).

3.1.1 Cluster of Excellence "Image Knowledge Gestaltung. An Interdisciplinary Laboratory"

(Period of funding 11/2012-10/2017)
Spokesmen: Prof. Dr. Horst Bredekamp and
Prof. Dr. Wolfgang Schäffner (both HU)
www.interdisciplinary-laboratory.hu-berlin.de

Science can be viewed as a "Gestaltung" of all its elements, from the laboratory arrangement of the chemical formula and the outline of a study to the theory building. Since time immemorial, knowledge has been designed by architectures, tools and models, and information tools and images. With the development of digital imaging methods, the importance of Gestaltung for the production and perception of knowledge has reached a new level for well over a half century. As a means for visualization and compression, modeling and mediation, evidence, and archiving images have caused a profound change in the sciences and humanities, technology, and medicine. They make vast amounts of data and complexities understandable. By no means are they effective only immaterially, but rather fold the digital and the material, because they are a comprehensive reservoir of forms of knowledge. Images open disciplinary boundaries and transport local styles and aesthetic strategies.

"Gestaltung", a paradigm from modern design and production processes, has been moved from the periphery to the core of the research itself. The cluster "Image Knowledge Gestaltung", in which images and knowledge are explored as design processes, plays a key role here. Furthermore, an interdisciplinary laboratory has been established as a new virtual and physical architecture of knowledge. The humanities, the sciences, and technology as well as the design disciplines have been brought together. "Gestaltung" has become a model in terms of scientific activity. With the participation of 22 disciplines from numerous university and non-university research institutions and museums, an integrative scientific platform has been formed that could change the Humboldt-Universität in a striking manner.

The scholars and scientists participating in the project come from a wide range of institutions: Humboldt-Universität, Technische Universität Berlin, Berlin University of the Arts, the Max Planck Institute of Colloids and Interfaces, the Max Planck Institute for the History of Science, the Ibero-American Institute, the Museum of Decorative Arts, the Bauhaus Dessau Foundation, Berlin Weißensee School of Art, the Museum für Naturkunde

(Natural History Museum), the Art Library, Federal Institute for Materials Research and Testing, and the Center for Literary and Cultural Research.

Participating IRIS members:

- Prof. Dr. Jochen Brüning
- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe
- Prof. Dr. Matthias Staudacher

3.1.2 Cluster of Excellence "Unifying Concepts in Catalysis - UniCat"

(Period of funding 11/2007-10/2017)
Spokesman: Prof. Dr. Matthias Drieß (TU Berlin)
www.unicat.tu-berlin.de

More than 50 research groups from chemistry, physics, biology, and engineering from the Technische Universität Berlin (coordinating university), the Freie Universität Berlin, Humboldt-Universität zu Berlin, the University of Potsdam, the Fritz-Haber-Institut der Max-Planck-Gesellschaft, and the Max-Planck Institute of Colloids and Interfaces in Potsdam work in the cluster of excellence "UniCat" on the research and development of catalysts. This cluster is unique in Germany, as it combines a wide range of scientific expertise with modern methods of engineering sciences, which in turn allows optimal conditions for the development of new catalytic processes.

Three major areas are linked in this concept: The development and research of catalysts are carried out by both classical chemistry and the biological and materials sciences. The implementation of results into industrial applications requires engineers from different disciplines. These researchers present their results to potential users in demonstration projects, so-called Mini-Plants, after showing the technical and economic viability of the newly developed method. Embedded in the organizational structure of "UniCat" is the "Berlin International Graduate School of Natural Sciences and Engineering" (BIG-NSE), which was established in May 2007 at the Technische Universität Berlin. The Graduate School is to enable new synergies for a structured doctoral training. The BIG-NSE sees itself as a magnet for young, internationally successful early-stage scientists and scholars from the sciences and engineering.

Participating IRIS members:

- Prof. Dr. Christian Limberg
  Prof. Dr. Joachim Sauer

3.1.3 Berlin Mathematical School

(Period of funding 11/2007-10/2017)
Spokesman: Prof. Dr. Jürg Kramer (HU)
www.math-berlin.de

In the Berlin Mathematical School (BMS) mathematics professors provide promising young scientists an excellent graduate education. The BMS that was initiated by excellent scientists from Humboldt-Universität zu Berlin, Freie Universität Berlin, and Technische Universität Berlin reaches out to graduates with a master's or bachelor's degree in mathematics who want to do a doctorate in a structured and closely supervised program. Therefore the school offers training in two phases that combine the strengths of German doctoral training with the merits of successful U.S. graduate schools. The concept of the graduate school is as follows: Phase I lasts for 3 to 4 semesters and offers a program of lectures in seven research areas that reflect the strengths of the three mathematics institutes. These include analysis, geometry, and mathematical physics, algebra and number theory, stochastics and financial mathematics, discrete mathematics and optimization, visualization and geometry processing, numerical mathematics and scientific computing, mathematical modelling, and applied analysis.

During Phase I, the students are given a broad mathematical training that lays the foundation for their future specialization. The classes are held at the three participating universities, and teaching takes place on different days at each university. One advantage for the graduates of Phase I is that, like in the U.S. graduate system, they do not need to do a master's degree. Phase II, which takes four to six semesters, begins immediately after an oral examination. As a rule, the students engage in research in one of Berlin's four DFG Research Training Groups in mathematics, or one of two International Max Planck Research Schools in Berlin that cooperate with the BMS.

Participating IRIS members:

- Prof. Dr. Jochen Brüning
- Prof. Dr. Jürg Kramer
- Prof. Dr. Dirk Kreimer
- Prof. Dr. Matthias Staudacher

3.1.4 School of Analytical Sciences Adlershof SALSA

(Period of funding 11/2012-10/2017)
Spokespersons: Prof. Dr. Janina Kneipp (HU) and
Prof. Dr. Ulrich Panne (Federal Institute for Materials Research and Testing & HU)
www.salsa.hu-berlin.de

Analytical chemistry is positioned in a rather fluid zone between the other natural sciences. For example, tools from physics and biochemistry often need to be employed. The SALSA Graduate School’s aim is to add new impetus to the analytical sciences by taking an interdisciplinary approach to teaching and research, by setting up a new curriculum, and through the close collaboration of experts from the fields of analytical and physical chemistry, biology, physics, statistics, modelling, and educational science.

The Graduate School is part of "Analytic City Adlershof", a competence center that bundles the university, non-university, and industrial expertise available at the Adlershof site in order to focus on questions and problems related to analytical chemistry. A bilateral partnership will be established with the Eidgenössische Technische Hochschule Zürich with the aim to foster scientific exchange and develop a joint "Curriculum in Analytical Sciences".

Participating IRIS members:

- Prof. Dr. Matthias Ballauff
- Prof. Dr. Oliver Benson
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Norbert Koch
- Prof. Dr. Christian Limberg
- Prof. Dr. Jürgen P. Rabe

3.2 Collaborative Research Centers (CRC)

3.2.1 CRC 647 "Space-Time-Matter: Analytic and Geometric Structures"

(Period of funding: 01/2005 – 12/2016)
Spokesmen:
Prof. Dr. Jochen Brüning (HU) (until 12/2014)
Prof. Dr. Matthias Staudacher (HU) (since 12/2014)
www.raumzeitmaterie.de

The CRC 647 is located in the core content of the IRIS research area "Space-Time-Matter". Scientists from mathematics and physics address here questions of geometric analysis, differential geometry, string theory and cosmology.

The projects dealt with can be divided into two major groups: group A investigates the geometry of matter, and group B is concerned with the evolution of geometric structures. Each group deals with five projects with both mathematicians and physicists contributing to the solution of interdisciplinary problems.

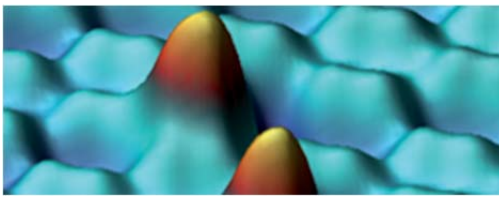
At the CRC are involved: the Humboldt-Universität as coordinating university, the Freie Universität, the University of Potsdam and the Max Planck Institute for Gravitational Physics / Albert Einstein Institute (AEI) in Golm.

Participating IRIS members:

- Prof. Dr. Jochen Brüning
- Prof. Dr. Dirk Kreimer
- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

3.2.2 CRC 658 "Elementary Processes in Molecular Switches at Surfaces"

(Period of funding: 07/2005 – 06/2017)
Spokesman: Prof. Dr. Felix von Oppen (FU Berlin)
www.physik.fu-berlin.de/sfb658



The increasing miniaturization and integration in electronic devices and sensors opens the perspective to use molecules as building blocks for functional molecular nanostructures. For applications like molecular electronics it will be essential to control the switching between different molecular states which in nature is often realized by photoinduced conformational changes.

Controlled switching of molecular function requires the synthesis and design of appropriate molecular nanosystems and a basic understanding of structural and electronic properties including the interaction with the environment. In addition there is a demand for active control by external stimuli like electromagnetic fields, forces and currents. The inter-action of molecules with surfaces opens new perspectives: It allows to assemble molecules with defined orientations and to vary the lateral couplings in a systematic manner. The contact of molecules to solid state interfaces is also essential to connect the molecular system with the outside world, in particular for electric transport.

Participating IRIS members:

- Prof. Dr. Claudia Draxl
- Prof. Dr. Thomas Elsässer
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Jürgen P. Rabe

3.2.3 CRC 765 "Multivalency as a Chemical Principle of Organization and Effectiveness: New Architectures, Functions and Applications"

(Periods of funding: 01/2008 – 12/2015)
Spokesman: Prof. Dr. Rainer Haag (FU Berlin)
www.sfb765.de

Multivalency is of vital significance in the (self)-organization of matter, in cognitive processes and signal transduction going on in biological systems. Thus, the development of new multivalent molecules is of great importance for approaching major biological issues such as the inhibition of inflammatory processes and the prevention of viral infections as well as for the systematical production of functional molecular architectures.

Participating IRIS members:

- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Jürgen P. Rabe

3.2.4 CRC 787 "Semiconductors - Nanophotonics: Materials, Models, Construction Components"

(Period of funding: 01/2008 – 12/2015)
Spokesman: Prof. Dr. Michael Kneissl (TU Berlin)
www.sfb787.tu-berlin.de

The Collaborative Research Center 787 "Semiconductor nanophotonics: materials, models, devices" combines three complementary areas of research aiming at the development of novel photonic and nanophotonic devices. The close collaboration between the different research areas and their mutual integration help explore new functionalities of nanophotonic devices and open new dimensions of applications. These include quantum key systems that are based on q-bit and entangled photon emitters, high frequency vertical cavity surface emitting lasers for future multi-terabus systems, quantum dot lasers, and optical amplifiers for ultra-high bit rate Ethernet, as well as high brilliance IR and visible lasers for materials processing and laser displays. The CRC 787 comprises a total of 17 projects from TU Berlin, which is also the speaker university, the Humboldt Universität zu Berlin, the Otto-von-Guericke University Magdeburg as well as the Ferdinand-Braun-Institut (Leibniz Institut für Höchstfrequenztechnik), the Fraunhofer-Institut für Nachrichtentechnik (Heinrich-Hertz-Institute), the Weierstraß-Institute for Applied Analyis and Stochastic, and the Konrad-Zuse-Zentrum für Informationstechnik.

Participating IRIS member:

- Prof. Dr. Oliver Benson

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

(Period of funding: 07/2011 – 06/2015)
Spokesman: Prof. Dr. Fritz Henneberger (HU) († 2015)
www.physik.hu-berlin.de/sfb951

The Collaborative Research Center HIOS is an interdisciplinary effort to bring together scientists with complementary expertise from three universities and four non-university institutions. The goal is the merger of inorganic semiconductors, conjugated organic materials, and metal nanostructures into novel hybrid structures. Elucidating and tailoring the fundamental chemical, electronic, and photonic interactions in these systems will enable us to develop functional elements exhibiting superior opto-electronic functionalities that are not achievable with any of the individual materials classes alone. The CRC 951 HIOS is a joint research project by scientists of Humboldt-Universität (coordinating university), the Technische Universität Berlin, the University of Potsdam (UP), the Helmholtz-Zentrum Berlin, the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI), the Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI), and the Paul-Drude-Institut für Festkörperelektronik (PDI).

CRC 951 is a central part of the IRIS research area "Hybrid Systems for Optics and Electronics".

Participating IRIS members:

- Prof. Dr. Matthias Ballauff
- Prof. Dr. Oliver Benson
- Prof. Dr. Claudia Draxl
- Prof. Dr. Thomas Elsässer
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Fritz Henneberger († 2015)
- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

3.2.6 CRC 1109 "Understanding of Metal Oxide/Water Systems at the Molecular Scale: Structural Evolution, Interfaces, and Dissolution"

(Period of funding: 04/2014 – 12/2017)
Spokesman: Prof. Dr. Christian Limberg (HU)
www.chemie.hu-berlin.de/forschung/sfb1109

The Collaborative Research Center 1109 is an interdisciplinary research platform that brings together scientists from four universities and three non-university institutions. It comprises 18 research projects which are led by 23 principal investigators (PIs) with diverse expertise in chemistry and physics.

The research aims at a comprehensive understanding of the complex atomic scale processes underlying oxide formation, structural evolution, and dissolution. Exemplarily, silica, alumina, and iron oxides will be studied as metal oxides with the highest natural abundance and application relevance. The long-term research results will be useful for reaching a rational synthesis of oxides with desirable properties, such as stability towards corrosion.

Participating IRIS members:

- Prof. Dr. Christian Limberg
- Prof. Dr. Joachim Sauer

3.3 7th Framework Program of the European Commission (FP 7)

3.3.1 HYMEC

"Hybrid organic/inorganic memory elements for integration of electronic and photonic circuitry"
(Period of funding: 10/2011 – 09/2014)
Coordinator: Prof. Dr. Norbert Koch (HU & HZB)
hymec2.physik.hu-berlin.de

Since October 2011 Prof. Norbert Koch has been coordinating the EU research project "Hybrid Organic/Inorganic Memory Elements for Integration of Electronic and Photonic Circuitry" (HYMEC), which was promoted for three years with € 3 million by the 7th EU Framework Program.

The objectives of "HYMEC" are to resolve fundamental issues of materials science and to realize new hybrid inorganic/organic devices with functionality far beyond the current state-of-the-art. This is directly relevant for the objectives of the FP7-NMP Work Program, as its goal is to "design novel knowledge-based smart materials with tailored properties, releasing their potential for enhanced and innovative applications". Specifically, the participating scientists have been performing research towards understanding and controlling all relevant properties of systems comprising inorganic metal nanoparticles embedded in matrices of conjugated organic materials (organic semiconductors). They also have been demonstrating the function of such material hybrids as non-volatile memory elements that can be addressed electrically and optically, which thus represent potential interconnects for future hybrid electronic and photonic circuitry.

In addition to the Humboldt-Universität, there other participating universities and non-university research institutions in Belgium, Germany, Italy, Austria, France, and Poland in the project as well as a technology-oriented company.

Participating IRIS member:

- Prof. Dr. Norbert Koch

3.3.2 GENIUS

"Graphene-Organic Hybrid Architectures for Organic Electronics: A Multisite Training Action"
(Period of funding: 12/2010 - 11/2014)
Coordiniator: Dr. Vincenzo Palermo
(Consiglio Nazionale delle Ricerche, Italien)
www.genius-network.eu

GENIUS is a multi-site ITN (Initial Training Network) aimed at enabling supra-sectorial and cross-disciplinary training and research in an emerging field at the interface between Supramolecular Chemistry, Materials Science, Nanoscience, Physics, and Engineering. The overall mission of GENIUS is to improve the career perspectives of early-stage researchers (ESRs) and a few experienced researchers (ERs) in both the public and private sector in the societal and economically important area of organic electronics and nanotechnology. To this end, we have set up an 8-partner joint training program to enable a pool of young researchers to gain expertise in the area of supramolecular materials, while simultaneously generating new scientific and technological knowledge relevant to industry.

The main objective of GENIUS is to train a new generation of young researchers in the production, processing, and characterization of graphene, the most recent and very promising nanotechnology breakthrough. The main goal of the project is to guide a new generation of young researchers in its production, processing, and characterization.

- Organic and supramolecular synthesis
- Advanced top-down and bottom-up nanofabrication techniques to self-assemble the GOHs in solution and on surfaces
- Scanning Force Microscopy (SFM) characterization of physico-chemical properties of the GOHs
- New computational techniques to model graphenic systems
- Steady-state and time-resolved spectroscopies both in solution and solid state, fabrication and testing of graphene-based devices
- Development of new composites of technological interest for application in the fields of electronics and consumer products

Participating IRIS members:

- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

3.3.3 AtMol

"Atomic Scale and Single Molecule Logic Gate Technologies"
(Period of funding: 12/2010 - 12/2014)
Spokesman: Prof. Dr. Christian Joachim
(Centre National de la Recherche Scientifique, Toulouse, Frankreich)
www.atmol.eu

A group of chemists focused on organic synthesis and headed by IRIS member Professor Stefan Hecht developed molecular building blocks for the production of single molecular wires in the project "Atomic Scale and Single Molecule Logic Gate Technologies (ATMOL)". The goal is to realize a first prototype for molecule-based computer chips.

In this project, nanowires modeled by the Hecht Group were examined in collaboration with the Fritz-Haber-Institut for their electrical conductivity. After successful production and testing, these molecular circuits were contacted by other scientists with tiny nano-electrodes and ultimately be packaged in a complete molecular chip. The project, in which an international consortium of scientists and engineers has already been cooperating for four years, has been funded by the European Union with 10 million euros.

Participating IRIS member:

- Prof. Stefan Hecht, Ph.D.

3.3.4 GATIS

"Gauge Theory as an Integrable System"
(Period of funding: 01/2013 - 12/2016)
Coordinator: Prof. Dr. Volker Schomerus
(Deutsches Elektronen-Synchrotron DESY)
gatis.desy.eu

GATIS is a multi-initial training network on gauge theory as an integrable system. Gauge theories provide the most successful framework for the description of nature particularly of high energy physics. However, extracting reliable and relevant predictions for gauge theory experiments has remained a major challenge, partly because they require a massive use of computer algebra. Over the last decade, an entirely new approach to quantum gauge theories has begun to emerge, initiated by a celebrated duality between gauge and string theory. This has brought an area of science into gauge theory that seemed unrelated a few years before, namely, the theory of low-dimensional statistical systems and strongly correlated electron systems. The paradigm governing this view point is "Gauge theory as an integrable system". The partners of this network derive from different areas of gauge theory, statistical physics, and computer algebra. With the proposed Initial Training Network, the initiators will carry the emerging multidisciplinary interaction to an entirely new level and bridging the gaps between our research areas in the context of graduate training activity. We believe that a coordinated education of young scientists in all the tools under development from the different communities offers tremendous potential for progress in the understanding and application of gauge theory. A group of carefully selected private sector partners are assisting the dissemination of results, methods, and ideas into neighboring scientific disciplines as well as to the general public. At the same time, they will also be vital in preparing the early-stage researchers for active and leading roles in academia and beyond.

Participating IRIS members:

- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

3.4 Graduate Schools and Master Program

Within the wide range of their research projects, the members of **IRIS Adlershof** are involved in training highly qualified young scientists.

3.4.1 Research Training Group 1324 METRIK

"Model-Based Development of Technologies for Self-Organizing Information Systems for Application to Disaster Management"
(Period of funding: 04/2006-03/2015)
Spokesman: Prof. Dr. Joachim Fischer (HU)
metrik.informatik.hu-berlin.de

The scientists in METRIK work on wireless sensor networks without a lavish central administration and wiring technology, have low costs regarding construction and electricity consumption, and operate under the principle of self-organization. These novel infrastructures of communication are being investigated because they could be applied as early warning systems for earthquakes and used in monitoring and information systems.

Participating IRIS members:

- Prof. Johann-Christoph Freytag, Ph.D.
- Prof. Dr. Alexander Reinefeld

3.4.2 Research Training Group 1504 "Mass, Spectrum, Symmetry"

"Particle Physics in the Era of the Large Hadron Collider"
(Period of funding: 04/2009 - 03/2018)
Spokesmen: Prof. Dr. Jan Plefka (HU) (until 09/2013)
Prof. Dr. Heiko Lacker (HU) (since 09/2013)
www.masse-spektrum-symmetrie.de

While working in this group, doctoral students familiar with experimenting, on the one hand, or with theory, on the other, will become acquainted with the sphere of research they are not used to. For the experimenting contingent, there will primarily be research work at the Atlas Detector of the LHC. Besides the astrophysical groups conducting the IceCube experiments in the Antartic and H.E.S.S., researchers are involved in Namibia. The theoretical physicists, in turn, whose common denominator is the quantum field theory, are working to find new approaches reaching beyond the standard model.

The challenges emerging from the LHC require a strong integration and communication of the different experimental and theoretical working areas of elementary particle physics, which is precisely the key goal of this research training group. Furthermore, they aim to unify the broad experimental and theoretical expertise in Berlin, Dresden, and Zeuthen and to place the common character of elementary particle physics back into the center of the doctoral students' training. The common link between the involved experimental groups is their participation in the ATLAS experiment at LHC and the search for new physics there. The link between the theoretical groups that are in the cooperation is quantum field theory, which is treated perturbatively, nonperturbatively, numerically, and generally in the context of string theory.

In addition to the broad spectrum of the participating research groups, which is unique for the eastern part of Germany, the research training group is characterized by a large number of participating junior researchers.

The curriculum is geared for excellent doctoral students, who will be trained in lectures and seminars at the Humboldt University and the Technical University of Dresden as well as in weekly intensive courses on topics in elementary particles that take place twice a year. Further features of the research training group are a secondary advisor concept, a midterm report, as well as a fast track to a PhD opportunity for excellent Master's students.

Participating IRIS members:

- Prof. Dr. Dirk Kreimer (associated faculty member)
- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

3.4.3 International Research Training Group 1524

"Self-Assembled Soft Matter Nano-Structures at Interfaces"
(Period of funding: 04/2009-09/2016)
Spokesman: Prof. Dr. Martin Schoen (TU Berlin)
www.ssni.tu-berlin.de

SSNI

The International Graduate Research Training Group is aiming at fundamental properties of self-assembled nanostructures of soft (organic and biomolecular) matter at interfaces. The studies are devoted to the nature of the structures formed and the driving forces behind their formation. A common objective of the research program is a better understanding of the interplay of the length scales characterizing the substrate and the properties of the self-assembled surface structures formed at the substrate. Research will be focused on three types of systems of different degree of complexity: (i) Systems in which the characteristic length scale results from a surface pattern imposed on an otherwise flat solid surface. Specifically, it will be investigated how ''chemical'' patterns ranging from nano- to micrometer dimensions can be formed through self-assembly and how they can be imprinted onto adjacent soft-matter phases. (ii) Systems with curved interfaces, in which the mean radius of curvature of the substrate represents a primary length scale. The self-assembly of amphiphilic molecules at the surface of colloidal particles into surface micelles, bilayers, etc. is an example of such systems. (iii) Biomimetic structures of various length scales within interfaces. Typical issues here are, for example, the size and stability of domains formed in multicomponent biomembranes or field-induced pattern formation of colloidal particles at interfaces.

Participating IRIS members:

- Prof. Dr. Matthias Ballauff
- Prof. Dr. Regine von Klitzing
- Prof. Dr. Jürgen P. Rabe

3.4.4 Research Training Group 1651 SOAMED

"Service-Oriented Architectures for the Integration of Software-Based Processes as Demonstrated by the Example of the Health Service and Medical Technology"
(Period of funding: 04/2010-09/2019)
Spokesman: Prof. Dr. Wolfgang Reisig (HU)
www.ki.informatik.hu-berlin.de/soamed

In this graduate school, doctoral students investigate software components which are to support and, at least partly, control communication in a complex network consisting of human beings, medical technology, data systems, and medical organizations. Their research aims to increase the efficiency and reduce the cost of the health service. The Humboldt-Universität zu Berlin, the Technische Universität Berlin, the Charité Berlin, and the Hasso-Plattner-Institut Potsdam are involved in this graduate program.

Participating IRIS member:

- Prof. Johann-Christoph Freytag, Ph.D.

3.4.5 International Research Training Group 1740

"Dynamical Phenomena in Complex Networks: Fundamentals and Applications"
(Period of funding: 10/2011-03/2016)
Spokesman: Prof. Dr. Jürgen Kurths (HU)
www.physik.hu-berlin.de/irtg1740

The focus within this first German-Brasilian research training group is on Amazonia, the rainforest, and a better understanding of partial systems on earth in continuously changing conditions. The investigations are concentrated on the consequences which the deforestation of the area around the Amazon has on the region as a whole as well as on the climate worldwide, with different options for further development.

Participating IRIS member:

- Prof. Dr. Fritz Henneberger († 2015)

3.4.6 International Research Training Group 1800

"Moduli and Automorphic Forms:
Arithmetic and Geometric Aspects"
(Period of funding: 07/2012-12/2016)
Spokesman: Prof. Dr. Jürg Kramer (HU)
www.mathematik.hu-berlin.de/~grk1800

The profile of the new international research training group "Combining and Interconnecting the Extensive Expertise in Arithmetic Algebraic Geometry and Complex Geometry" is the goal of International Research Training Group 1800 "Moduli and Automorphic Forms: Arithmetic and Geometric Aspects". Its early-career researchers are especially interested in examining the interplay between the arithmetic and the geometry of moduli spaces as well as problems in the theory of automorphic forms. The research program encompasses the three research areas of arithmetic moduli, heights and densities, degenerations, and automorphic forms, which are mutually interconnected. Humboldt-Universität zu Berlin cooperates with the University of Leiden and University of Amsterdam in the Netherlands.

Participating IRIS member:

- Prof. Dr. Jürg Kramer

3.4.7 International Max Planck Research School

"Functional Interfaces in Physics and Chemistry"
Spokesman: Prof. Dr. Martin Wolf
(Fritz-Haber-Institut der Max-Planck-Gesellschaft)
www.imprs-cs.mpg.de

The physical and chemical properties of material surfaces play an important role in many large scale applications, such as in heterogeneous catalysis and corrosion inhibition. With the shrinking dimensions of electronic and optoelectronic devices, surface properties are becoming increasingly important in many fields of modern technology, such as in thin film growth. In this emerging field, which combines electronic devices with biological applications, the surface properties dominate such issues as biocompatibility. The last two decades have seen a rapid progress in our understanding of fundamental processes on highly idealized surfaces.

The International Max Planck Research School on "Functional Interfaces in Physics and Chemistry" aims at combining the expertise of several strong research groups at the Humboldt Universität zu Berlin, the Freie Universität Berlin, and the Fritz-Haber-Institut der Max-Planck-Gesellschaft in order to create a unique opportunity for foreign and German students in terms of cutting-edge research and a thorough training in the methods, concepts, and theoretical basis of the physics and chemistry of surfaces. The research school provides an interdisciplinary environment, and a wealth of methods using state-of-the-art equipment.

Participating IRIS members:

- Prof. Dr. Claudia Draxl
- Prof. Dr. Norbert Koch
- Prof. Dr. Joachim Sauer

3.4.8 International Max Planck Research School

"Multiscale Bio Systems"
Spokesman: Prof. Dr. Reinhard Lipowsky
(Max Planck Institute of Colloids and Interfaces)
imprs.mpikg.mpg.de

The IMPRS on Multiscale Bio Systems addresses the fundamental levels of biosystems as provided by macromolecules in aqueous solutions, molecular recognition between these building blocks, free energy transduction by molecular machines, as well as structure formation and transport in cells and tissues. The research activities are focused on four core areas:

- Molecular recognition of carbohydrates
- Interaction of biomolecules with light
- Directed intracellular processes
- Directed shape changes of tissues.

One general objective is to understand, in a quantitative manner, how the processes on supramolecular and mesoscopic scale between a few nanometers and many micrometers arise from the structure and dynamics of the molecular building blocks. To achieve this goal, our interdisciplinary research combines bottom-up with top-down approaches, which are pursued by several groups from theoretical and experimental biophysics, from physical and colloid chemistry, as well as from biochemistry and molecular biology.

The IMPRS on Multiscale Bio-Systems involves the Max Planck Institute of Colloids and Interfaces, which is the main organizational structure, the University of Potsdam, the Freie Universität and the Humboldt-Universität zu Berlin as well as the Fraunhofer Institute for Biomedical Engineering IBMT.

Participating IRIS members:

- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Jürgen P. Rabe

3.4.9 International Max-Planck Research School

"Geometric Analysis, Gravitation and String Theory"
(Period of funding: 01/2004-12/2015)
Spokesman: Prof. Dr. Hermann Nicolai
(Max Planck Institute for Gravitational Physics)
www.aei.mpg.de

The International Max Planck Research School (IMPRS) for "Geometric Analysis, Gravitation, and String Theory" aims to promote research in mathematical physics in an area related in the widest sense to Einstein's theory of general relativity, ranging from pure mathematics (differential geometry and the theory of partial differential equations) to the physics of black holes, gravitational waves, and cosmological applications of Einstein's theory, and all the way to the most recent efforts to reconcile Einstein's theory with quantum mechanics in the framework of superstring theory and M theory. The school started operating in January 2004.

Students enroll in a doctoral program at one of the participating universities. Every student is assigned a primary and a secondary adviser by the executive committee. In addition to their research work, students are expected to attend advanced lecture courses that are offered by the school. Moreover they are required to present progress reports of their work in regular intervals at local seminars. The program, dissertation, and exams are in English or German. The PhD should be completed within 2-3 years.

Participating IRIS members:

- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

3.4.10 Graduate School Hybrid4Energy

"Hybrid Materials for Efficient Energy Generation and Information Technologies"
(Period of funding: 04/2014-03/2017)
Spokesman: Prof. Dr. Norbert Koch (HU & HZB)
www.physik.hu-berlin.de/h4e

Hybrid4Energy, a graduate school for Hybrid Materials for Efficient Energy Generation and Information Technologies, is a joint venture of Humboldt-Universität zu Berlin and the Helmholtz-Zentrum Berlin für Materialien und Energie GmbH.

The program offers a structured, three-year period of multidisciplinary research combined with an integrated curriculum in physics and chemistry.

The objective of this graduate school is to push interdisciplinary education, training, and research on hybrid organic/inorganic systems for electronic, optoelectronic and photovoltaic devices. The Campus Adlershof with its wide range of expertise allows doctoral students to grow and benefit from an excellent interdisciplinary environment and research facilities. The research program focuses on unravelling the electronic, optoelectronic, and photonic properties of organic/inorganic hybrid systems in a concerted experimental and theoretical approach studied, with the goal of predicting and controlling the material properties and functionalities. The knowledge gained will then be applied to the fields of renewable energy and next generation information technology.

Participating IRIS members:

- Prof. Dr. Oliver Benson
- Prof. Dr. Claudia Draxl
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Fritz Henneberger († 2015)
- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

3.4.11 Graduate School ProMINTion

(Period of funding: 11/2014-10/2017)
Spokespersons: Prof. Dr. Annette Upmeier zu Belzen
& Prof. Dr. Burkhard Priemer (both HU)
promint.hu-berlin.de/promintion

The topic "Measurement Processes and Handling of Data" is part of the day-to-day scientific practice in the academic disciplines of science, technology, engineering, and mathematics (STEM). Likewise, students in mathematics and natural sciences come intensely into contact with that same issue at school and university. Nevertheless, the topic has attracted little interest in both the field of subject-related pedagogical research as well as the research field of university pedagogy. In fact, it is rather the topic "experimentation" that dominates the scientific discussion in the field of the subject-specific pedagogies (formulating a hypothesis, planning an investigation, data analysis). However, conducting measurements, acquiring data as such, processing data as well as presenting them are hardly taken into account and still remain a desideratum for future educational research.

In the framework of their scientific training, the graduate students pursue a subject-related international training program "Measuring Processes and Handling of Data", which focuses on both the specific scientific discipline and the subject-specific pedagogies. This includes, among other things, a three-month professional internship in a research institute at Berlin-Adlershof. While the combination of scientific disciplines and subject-specific pedagogies is quite well-established in the university training programs for future STEM teachers, the systematic integration of the scientific disciplines (like systems biology, computer simulation, big data) is an innovation in the field of STEM pedagogy research.

In order to promote the internationalization of young scientists, the program "ProMINTion" includes a three-month international research stay in a subject-specific pedagogy research group. Moreover, "ProMINTion" PhD students attend and present results at international conferences and workshops and receive communication skills training as well as training in academic writing, which promotes the visibility of the STEM pedagogies.

Participating IRIS members:

- Prof. Dr. Oliver Benson
- Prof. Dr. Jürg Kramer

3.4.12 Master of Science in Polymer Science Program

Spokespersons: Prof. Dr. Jürgen P. Rabe (HU)
& Prof. Dr. Regine von Klitzing (TU Berlin)
polymerscience.physik.hu-berlin.de

Polymer science is an interdisciplinary area comprised of chemical, physical, engineering, processing, and theoretical aspects. It also has enormous impact on contemporary materials science. Its goal is to provide the basis for the creation and characterization of polymeric materials and an understanding for structure/property relationships. Polymer science is of increasing importance for everyone's daily life. Many modern functional materials, gears, and devices have polymers as integral parts. Not surprisingly, roughly 30% of all scientists in the chemical industry work in the field of polymers. Despite its importance today and potential for future economic growth, there is no adequate university-level study program for polymer science in Germany.

The Berlin-Brandenburg Polymer Society (Berlin-Brandenburgischer Verband für Polymerforschung eV) became aware of this misbalance and initiated a two-year Master of Science polymer program, which will start in the winter semester of 1999/2000. It was jointly designed by polymer scientists of the three Berlin universities, Freie Universität Berlin, Humboldt-Universität zu Berlin, Technische Universität Berlin, and the nearby Universität Potsdam with the goal in mind to be competitive with renowned polymer centers abroad. To make it more attractive to foreign students the program will be in English.

This challenging interdisciplinary program will benefit from the close proximity of several other Berlin and Potsdam scientific centers such as the institutes of the Max Planck, Fraunhofer, and Helmholtz Societies, as well as the BESSY II synchrotron. The universities are very well equipped with the most state-of-the-art technical equipment and laboratories, specialty workshops, large service units, and modern computer facilities. The work of the polymer scientists in charge of the Polymer Science program is internationally renowned and endowed by industry, state, and private grants and awards. Participating IRIS members:

- Prof. Dr. Regine von Klitzing
- Prof. Dr. Jürgen P. Rabe

3.5 More Coordinated Collaborative Projects

3.5.1 Funding by the Einstein Foundation Berlin

The Einstein Foundation Berlin is funding the joint project "ETERNAL - Exploring Thermoelectric Properties of Novel Materials" of **IRIS Adlershof** member and Einstein Professor Claudia Draxl, Department of Physics at Humboldt-Universität zu Berlin, together with Prof. Klaus Müller, TU Berlin, and Prof. Matthias Scheffler, Fritz-Haber-Institut, as well as the project "Gravitation and High Energy Physics" of **IRIS Adlershof** member Matthias Staudacher, professor at the Departments of Mathematics and Physics at Humboldt-Universität zu Berlin.

The Einstein Center for Mathematics Berlin (ECMath) is a platform for the consolidation of the collaborative mathematical excellence projects in Berlin, including the DFG Research Center Matheon, the Berlin Mathematical School (BMS), and the German Center for Teacher Education in Mathematics (DZLM), in an internationally visible framework, using the organizational structure of Matheon as a role model. ECMath establishes the institutional basis for innovative first-rate research in mathematics ranging from application-driven as well as theoretical basic research, education of young researchers, and professional development of scientists in academia, schools, and industry, up to the transfer of mathematical research results into industrial practice. ECMath commenced operations on January 1, 2013, with Matheon, DZLM, and BMS as its founding collaborative excellence centers. It is open to further large-scale mathematical collaborative research units. Prof. Jürg Kramer is a member of the Executive Board.

3.5.2 Helmholtz-Energy-Alliance

"Inorganic / Organic Hybrid Solar Cells and Techniques for Photovoltaics"
(Period of funding: 05/2012-04/2015)
Spokesman: Prof. Dr. Norbert Koch (HU & HZB)
www.helmholtz.de/helmholtz_zentren_netzwerke/helmholtz_energie_allianzen/hybrid_solarzellen

The Helmholtz-Zentrum Berlin, the Jülich Forschungszentrum, the Humboldt-Universität zu Berlin, the University of Potsdam, and the Freie Universität Berlin have founded together one of the three new energy alliances that have been launched by the Helmholtz-Gemeinschaft in 2012.

The aim of this energy alliance called "Inorganic/Organic Hybrid Solar Cells and Techniques for Photovoltaics" is to meet the urgent need for research on the rapid conversion of energy supply. The projects are funded by the Initiative and Networking Fund of the Helmholtz-Gemeinschaft for three years. The university partners also contribute their own funds. A continuation of the research for more than three years is planned.

This research area is focused on processes that have limited up to now the effective power generation in the solar cell at the interfaces between inorganic semiconductors and organic materials. In order to improve the effectiveness of such solar cell arrays, researchers are using nanostructures among other things. Inorganic nanoparticles and nanowires are placed in organic materials to also ensure a cost effective production of such synthetic methods. The embedding of organic semiconductor between inorganic nanorods is very promising as well.

Due to the Helmholtz energy alliance, ongoing activities are been strengthened in such an internationally leading center for research and development of innovative hybrid photovoltaic arises. The "Centre for Hybrid Photovoltaic" is jointly operated by the Helmholtz-Zentrum Berlin, the Forschungszentrum Jülich, the Humboldt-Universität zu Berlin, the Freie Universität Berlin, the Technische Universität Berlin, and the University of Potsdam in the Integrative Research Institute for the Sciences **IRIS Adlershof** and the Wilhelm-Conrad-Röntgen Campus of the HZB. This center virtually links, on the one hand, the activities of the partners and, on the other, is physical based at the Science and Technology Park Berlin-Adlershof. The Berlin Center of Competence Thin Film and Nanotechnology for Photovoltaics, PVcomB, is associated as another partner.

Participating IRIS members:

- Prof. Dr. Claudia Draxl
- Prof. Stephan Hecht, Ph.D.
- Prof. Dr. Norbert Koch
- Prof. Dr. Fritz Henneberger († 2015)
- Prof. Dr. Jürgen P. Rabe

3.6 Collaborative Projects in the Context of Mathematics and Science Teacher Education and Training

The STEM subjects (science, technology, engineering, and mathematic) suffer in schools from an increasing loss of acceptance. The result is a shortage of highly skilled labor in the scientific fields. The key to an improving STEM education is the education and training of STEM teachers. Therefore, the Deutsche Telekom Stiftung initiated in 2009 and 2011 two competitions that gave the German teacher education and training in the STEM subjects a strong impetus.

3.6.1 Humboldt-ProMINT-Kolleg

(Period of funding: 08/2010-07/2017)
Spokespersons: Prof. Dr. Burkhard Priemer (HU)
& Prof. Dr. Annette Upmeier zu Belzen (HU)
www.promint.hu-berlin.de

The Humboldt-ProMINT-Kolleg is a interdisciplinary institution established at Humboldt-Universität zu Berlin that cooperates with different types of schools, in particular, via the delegation of teachers, students, graduate students/PhDs, and professors working in the mathematics and science education sector as well as in basic research. The necessary requirements for an excellent and practice-oriented teacher education for the prospective Master of Education candidates are thus provided with a sustainable long-term effect.

For its reorganization concept of teacher education in mathematics and the sciences, Humboldt-Universität zu Berlin was one of the four German universities that successfully participated in the university competition for teacher education in mathematics and the sciences, initiated by Deutsche Telekom Stiftung in 2009. In a second phase of the project, which started in August 2013 and will last until 2017, the processes that were initiated at the universities will be institutionalized and expanded. From 2014 Humboldt-Universität and the Freie Universität will coordinate a national network focusing on "School labs for STEM Teacher Education and Training".

Participating IRIS member:

- Prof. Dr. Jürg Kramer

3.6.2 German Center for Teacher Education in Mathematics (DZLM)

(Period of funding: 10/2011-09/2016)
Director: Prof. Dr. Jürg Kramer (HU)
www.dzlm.de

The aim of the DZLM is sustained improvement of the the mathematics teacher education in Germany. A consortium of six German universities coordinated by the Humboldt-Universität won the competition of the Deutsche Telekom Stiftung. The Deutsche Telekom Stiftung is providing 5 million euros for five years.

The DZLM is focusing on the training of teachers from the elementary and secondary levels, who teach outside of their expertise or of their subject area. The center will initially focus on mathematics. A later extension to other STEM subjects is planned.

Beside the Humboldt-Universität zu Berlin, the consortium consists of the Freie Universität Berlin, the Deutsche Universität für Weiterbildung in Berlin, the Ruhr-Universität Bochum, the University of Duisburg-Essen, and the University of Paderborn. The concept of the university consortium provides, among other things, an online platform that informs mathematics teachers and teacher trainers of current developments in research and teaching and of appropriate information and materials. In addition, the establishment of a master training course for teacher trainers is planned.

Participating IRIS member:

- Prof. Dr. Jürg Kramer

4 Scientific Communication, Events and Public Relations

The scientific results from IRIS research are communicated to the international professional public, especially through presentations at national and international conferences and in peer-reviewed publications in high-ranking scientific journals. The invited lectures at international conferences and scientific articles in reviewed journals regularly clearly exceed the 100-per-year mark, which documents the high scientific output of IRIS's members.

IRIS Adlershof presents its scientific activities and results on its homepage and not only singles out publications but also scientific highlights *(www.iris-adlershof.de/de/Highlights.html)*. A commonly understandable presentation method was chosen to adequately address even the interested readers without expertise in the fields being discussed. In the report period, quite a few articles on **IRIS Adlershof** have appeared in the daily press and other generally accessible media that have documented the public's interest in IRIS's research (see *www.iris-adlershof.de/de/Medien.html).*

4.1 Selected Scientific Highlights

4.1.1 Modifying the ZnO Workfunction by Adsorption of F4TCNQ

Hybrid inorganic/organic semiconductor (HIOS) heterojunctions have opened up new opportunities for (opto-)electronic devices due to their potential for combining the favorable properties of two distinct material classes. A group around **IRIS Adlershof** member Prof. Norbert Koch employed molecular acceptor interlayers to tune the work function of the substrate and thus change the energy level alignment (ELA) between the Fermi-level of the substrate and the energy levels of an organic semiconductor. This allows one to adjust the ELA to favor, e.g., energy or charge transfer across the interface.

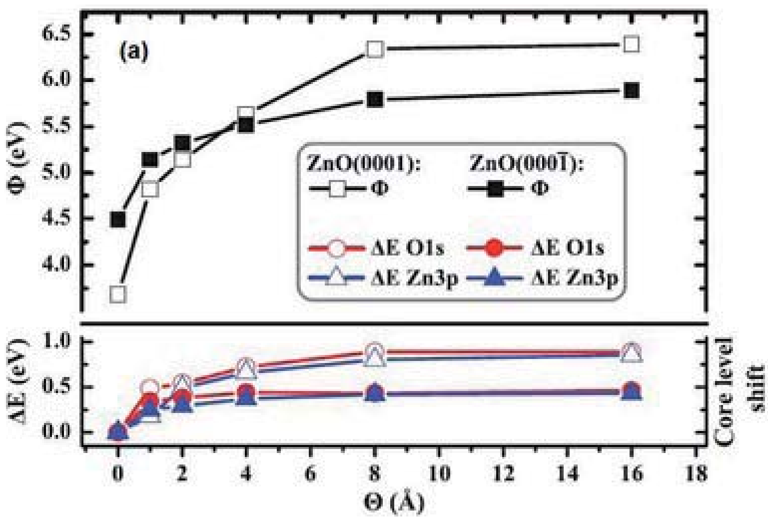
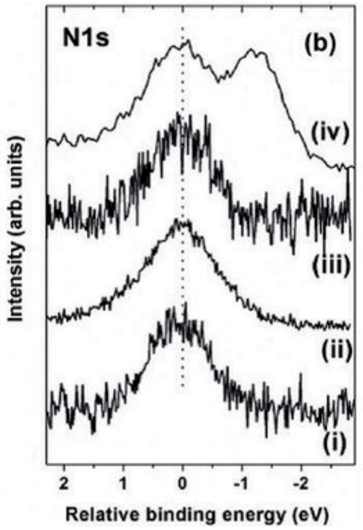


Fig.1: Evolution of the work function (Φ) as a function of F4TCNQ nominal thickness (Θ) on the ZnO(000-1)-O and ZnO(0001)-Zn surfaces and relative binding energy shifts ΔE of the O1s and Zn3p core levels upon adsorption of F4TCNQ.

The scientists demonstrated that the work function Φ of ZnO can be controlled over a wide range (up to 2.8 eV) by adsorbing the molecular electron acceptor F4TCNQ in the (sub-) monolayer regime. Although this is phenomenologically similar to what was observed for metal surfaces, the mechanism of the Φ increase markedly differs for the inorganic semiconductor.



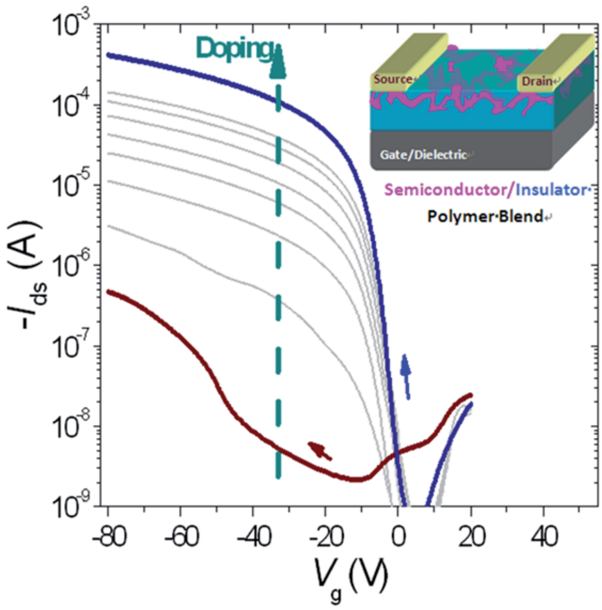
ΔΦ relies on two complementary mechanisms due to electron transfer to the surface-adsorbed acceptor, i.e., band bending in the inorganic semiconductor and an interface dipole, yielding $\Delta\Phi_{BB}$ and $\Delta\Phi_{ID}$, respectively (see Fig. 1). It was found that minute electron transfer is sufficient to induce significant ΔΦs (see Fig. 2).

Fig. 2: N1s core-level spectra of (i) 0.5-Å F4TCNQ on ZnO(0001), (ii) 8-Å F4TCNQ on ZnO(0001), (iii) 0.5-Å F4TCNQ on ZnO(000-1), and (iv) 60-Å F4TCNQ on Au. The low-binding energy component in spectrum (iv) is from F4TCNQ chemisorbed on Au with a net electron transfer of approximately 0.3-0.4 eV.

Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor
R. Schlesinger, Y. Xu, O. T. Hofmann, S. Winkler, J. Frisch, J. Niederhausen, A. Vollmer, S. Blumstengel, F. Henneberger, P. Rinke, M. Scheffler, and N. Koch
Physical Review B 87 (2013) 155311
DOI: 10.1103/PhysRevB.87.155311

4.1.2 Moderate Doping Leads to High Performance of Semiconductor/Insulator Polymer Blend Transistors

Polymer transistors are being intensively developed for next-generation flexible electronics. Blends comprising a small amount of semiconducting polymer mixed into an insulating polymer matrix have simultaneously shown superior performance and environmental stability in organic field-effect transistors compared with the neat semiconductor. Here a group of scientists including Prof. Norbert Koch, a member of **IRIS Adlershof**, shows that such blends actually perform very poorly in the undoped state and that mobility and on/off ratio are improved dramatically upon moderate doping. Structural investigations show that these blend layers feature nanometer-scale semiconductor domains and a vertical composition gradient. This particular morphology enables a quasi three-dimensional spatial distribution of semiconductor pathways within the insulating matrix, in which charge accumulation and depletion via a



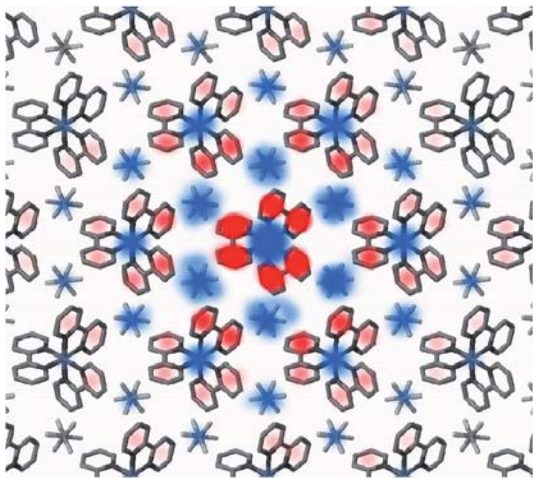
The effect of doping on the transistor performance of P3HT/PS blends and neat P3HT. In-situ evolution of the transfer characteristics (Vds= -5V, linear regime) on exposure time in 'dilute air' (N_2 atmosphere with O_2 concentration ~1 ppm and H_2O ~1 ppm). P3HT/PS (5% P3HT) gate bias is substantially different from neat semiconductor, and where high on-current and low off-current are simultaneously realized in the stable doped state. Adding only 5 wt% of a semiconducting polymer to a polystyrene matrix, the researchers realized an environmentally stable inverter with gain up to 60. This new approach promotes the OFET performance while providing a simple fabrication process. With this guidance, highly transparent transistors with field-effect mobilities comparable to that of amorphous silicon, combined with environmental stability and mechanical robustness, might become feasible.

Moderate doping leads to high performance of semiconductor/insulator polymer blend transistors
G. 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
Nature Communications 4 (2013) 1588
DOI: 10.1038/ncomms2587

4.1.3 Neighbors Move Electrons Jointly - An Ultrafast Molecular Movie on Metal Complexes in a Crystal

Applying femtosecond x-ray methods, researchers at the Max-Born-Institute in Berlin (Germany) and the École Polytechnique Federale de Lausanne (Switzerland) observed an extremely fast, collective electron transfer of ~100 molecular ions after excitation of a single electron in a crystal of transition metal complexes.

Photochemistry and molecular photovoltaics make frequent use of so-called transition metal complexes which consist of a central metal ion bonded to a group of surrounding ligands. Such materials display a strong absorption of ultraviolet or visible light, making them attractive as primary light absorbers in molecular solar cells and other devices of molecular optoelectronics. Absorption of light is followed by an extremely fast shift of electrons from the metal ion to the ligands, a mechanism that is essential for generating an electric voltage. All applications rely on solid-state materials in which transition metal complexes are densely packed and can interact with each other. So far, the influence of this interaction on the very fast electron motions following the absorption of light has remained unclear.



Cartoon of the collective charge transfer in $[Fe(bpy)_3]^{2+}(PF_{6-})_2$ which affects approximately 30 complexes around the directly photo-excited one. Blue: reduction of electron density, red increase of electron density.

To observe ultrafast electron motions in space and time, one needs to measure the position of electrons in the material with a precision of the order of 0.1 nm (0.1 nm $=10^{-10}$ m), roughly corresponding to the distance between neighboring atoms, and on a sub-100 fs time scale (1 fs = 10^{-15} s). This is possible by imaging the material with extremely short x-ray pulses that are scattered from the electrons and provide their spatial arrangement. The electron motions are initiated by an ultrashort optical pulse which excites an electron on an individual complex. In the *Journal of Chemical Physics* Benjamin Freyer, Flavio Zamponi, Vincent Juve, Johannes Stingl, Michael Wörner, **IRIS Adlershof** member Thomas Elsässer and Majed Chergui report the first in-situ x-ray imaging of electron and atom motions induced by such an electron transfer excitation. For the prototype material $[Fe(bpy)_3]^{2+}(PF_{6-})_2$, they show time-dependent 'electron maps' derived from x-ray snapshots taken with 100 fs long hard x-ray flashes. Taking x-ray snapshots at various times during and after the optical pulse that triggers the charge transfer creates a molecular movie of electron and atom motions.

To the big surprise of the researchers, the time-dependent 'electron maps' revealed a transfer of electronic charge not only from the Fe atoms to the bipyridine units but, which was so far unknown, to an even larger amount of electronic charge from the PF6- counterions to the bipyridine units. The analysis of the x-ray snapshots showed that the charge transfer affected approximately 30 complexes around the directly photo-excited one. This collective electron response is caused by the electric Coulomb forces between the different ions and minimizes the total electrostatic energy in the crystal. Such behavior is highly favorable for charge collection and injection in optoelectronic devices.

Ultrafast inter-ionic charge transfer of transition-metal complexes mapped by femtosecond X-ray powder diffraction
B. Freyer, F. Zamponi, V. Juvé, J. Stingl, M. Woerner, T. Elsaesser, and M. Chergui
Journal of Chemical Physics 138 (2013) 144504
DOI: 10.1063/1.4800223

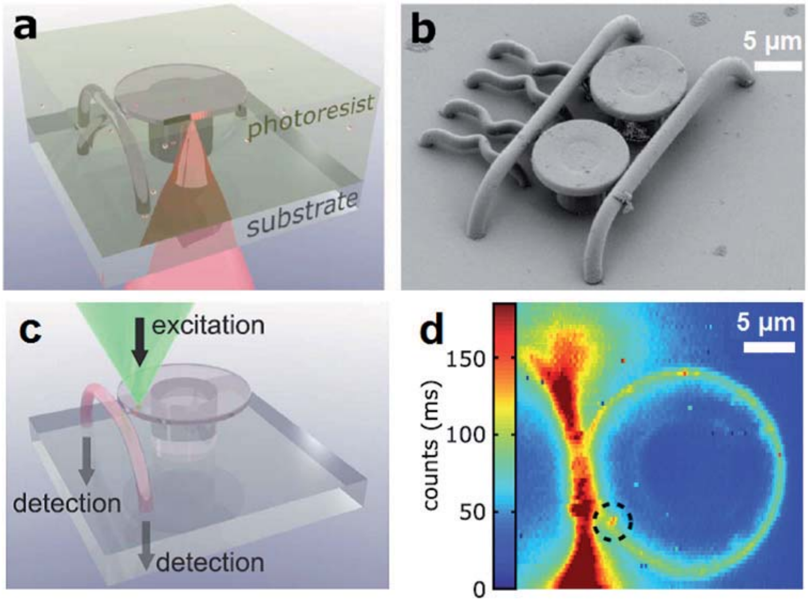
4.1.4 Quantum Light from Diamond and Plastic

A group of researchers led by **IRIS Adlershof** member Prof. Oliver Benson has developed a simple method for fabricating stable sources of single light quanta. The approach published in the Open Access Journal Scientific Reports of Nature Publishing Group is based on a novel hybrid approach combining two completely different material systems.

On the one hand, there are tiny fragments of diamond. Besides carbon, diamond contains other atoms as natural impurities. These impurity atoms or so-called color centers are responsible for the yellow or blue colors of natural diamond. Due to their very small size of only a few millionths of a millimeter, some of the diamond fragments contain only a single color center, which can be excited optically with the help of laser light. The color center releases its energy by emission of single quanta of light, or photons, which are thus generated one-by-one in a controlled way. The researchers then mixed the diamond fragments with a special photo resist.

A focused laser beam irradiating the resist layer induced local polymerization, i.e., the resist was turned into plastic. This way it was possible to nearly arbitrarily write three-dimensional structures that contained single diamond fragments with single color centers. The research team at first fabricated optical waveguides and resonators for an efficient collection and routing of the photons emitted from the color centers.

A major advantage of the new hybrid material system is, on the one hand, the well-established and cost efficient fabrication method and, on the other, the unlimited stability of operation even at room temperature. The next steps will be to combine the novel structures with other optical instrumentation. The researchers expect that numerous applications in



Figures: (a) Fabrication principle of optical disc resonators and bent waveguides using local polymerisation of a photoresist through a focussed laser beam. (b) Scanning electron microscopy image of a test structure. (c) Schematic of the generation and measurement of quantum light. A diamond fragment containing a single colour centre is excited optically by a laser. The emitted photons are collected by the resonator and coupled to the wave-guide. Detection is performed at the two ends of the waveguide. (d) Scanning fluorescence microscopy image of the structure shown in (c). A circle indicates the fluorescing diamond fragment.

the fields of high-resolution microscopy, optical sensing, or quantum information processing can be realized this way in a reliable and cost-efficient approach.

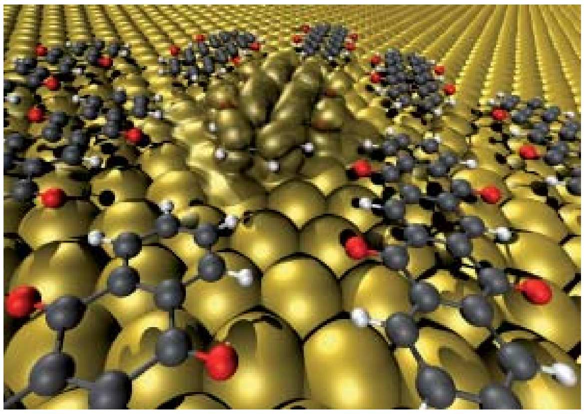
Three-dimensional quantum photonic elements based on single nitrogen vacancy-centres in laser-written microstructures
A. W. Schell, J. Kaschke, J. Fischer, R. Henze, J. Wolters, M. Wegener, and O. Benson
Scientific Reports 3 (2013) 1577:1-5
DOI: 10.1038/srep01577

4.1.5 Organic Electronics - How to Make Contact Between Carbon Compounds and Metals

Organic electronics has already hit the market in smart-phone displays and holds great promise for future applications like flexible electroluminescent foils (a potential replacement for conventional light bulbs) or solar cells that convert sunlight to electricity. A reoccurring problem in this technology is to establish good electrical contact between the active organic layer and metal electrodes. Organic molecules are also frequently used for this purpose. Until now, however, it was practically impossible to accurately predict which molecules performed well on the job. They basically had to be identified by trial-and-error. Now, an international team of scientists around Dr. Georg Heimel and Prof. Norbert Koch (**IRIS Adlershof**) from the HU and the HZB has unraveled the mystery of what these molecules have in common. Their discovery enables more focused improvements to contact layers between metal electrodes and active materials in organic electronic devices.

"We have been working on this question for a number of years now and could at last come up with a conclusive picture using a combination of several experimental methods and theoretical calculations", Georg Heimel explains. The researchers systematically examined different types of molecules whose backbones consist of the same chain of fused aromatic carbon rings. They differed in just one little detail: the number of oxygen atoms projecting from the backbone. These modified molecules were placed on the typical contact metals gold, silver, and copper.

Using photoelectron spectroscopy (UPS and XPS) at HZB's own BESSY II synchrotron radiation source, the researchers were able to identify chemical bonds that formed between the metal surfaces and the molecules as well as to measure the energy levels of the conduction electrons. Colleagues from Germany's Tübingen University determined the exact distance between the molecules and the metal surfaces using x-ray standing wave measurements taken at the ESRF synchrotron radiation source in Grenoble, France.



Upon contact between the oxygen atoms protruding from the backbone and the metal, the molecules' internal structure changed in such a way that they lost their semiconducting properties and instead adopted the metallic properties of the surface. (Visualization: Georg Heimel/HU)

These experiments showed that, upon contact between the oxygen atoms protruding from the backbone and several of the metals, the molecules' internal structure changed in such a way that they lost their semiconducting properties and instead adopted the metallic properties of the surface. Despite similar prerequisites, this effect was not observed for the "bare"-backbone molecule. From the observation which molecules underwent these kinds of drastic changes on what metal, the researchers could derive general guidelines. "At this point, we have a pretty good sense of how molecules ought to look like and what their properties should be if they are to be good mediators between active organic materials and metal contacts, or, as we like to call it, good at forming soft metallic contacts", says Heimel.

Experts from a number of other German universities and from research facilities in Suzhou (China), Iwate and Chiba (Japan), and ESRF (France) have also contributed substantially to this publication.

Charged and metallic molecular monolayers through surface-induced aromatic stabilization
G. Heimel, S. Duhm, I. Salzmann, A. Gerlach, A. Strozecka, J. Niederhausen, C. Bürker, T. Hosokai, I. Fernandez-Torrente, G. Schulze, S. Winkler, A. Wilke, R. Schlesinger, J. Frisch, B. Bröker, A. Vollmer, B. Detlefs, J. Pflaum, S. Kera, K. J. Franke, N. Ueno, J. I. Pascual, F. Schreiber, and N. Koch
Nature Chemistry 5 (2013) 187–194
DOI: 10.1038/nchem.1572

4.1.6 Space Charge Transfer in Hybrid Inorganic-Organic Systems

To describe charge transfer in hybrid inorganic/organic systems (HIOS), a first principles approach was developed, that explicitly includes the global effects of doping (i.e. position of the Fermi level) and the formation of a space-charge layer (see Fig. 1). For an example of tetrafluoro-tetracyanoquinodimethane (F4TCNQ) on the ZnO(000-1) surface (see Fig. 2), the group of Prof. Norbert Koch showed that the adsorption energy and electron transfer strongly depend on the ZnO doping.

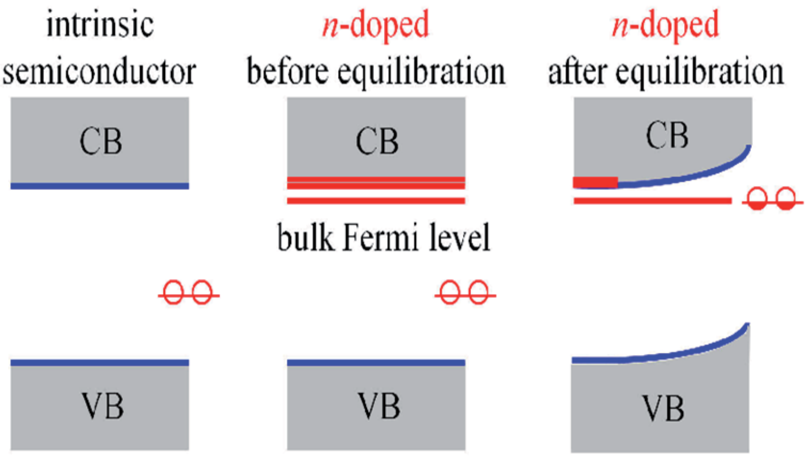


Fig.1: Schematic illustration of the electron transfer to acceptor states at a surface or interface of an n-doped semiconductor (middle and right). The development of a space-charge region induces band-bending, which brings the acceptor state closer to the Fermi level (right) In an undoped intrinsic semiconductor (left) no such electron transfer can take place resulting in an empty acceptor state in the band gap.

Figure 1 illustrates schematically how charge transfer proceeds. Initially, the empty acceptor state of F4TCNQ is situated below the Fermi level. Subsequently, the charge is transferred to the acceptor state and the resulting dipole lifts the state up to the Fermi level.

The dipole has two contributions: a short-ranged part arising from charge rearrangement at the surface (see Fig. 2 b) and a long-ranged part from the build up of a space-charge region. The latter is inversely proportional to the bulk doping concentration. For low doping concentrations, band bending alone can lift up the acceptor state to the Fermi level. This reduces the required electron transfer to nearly zero.

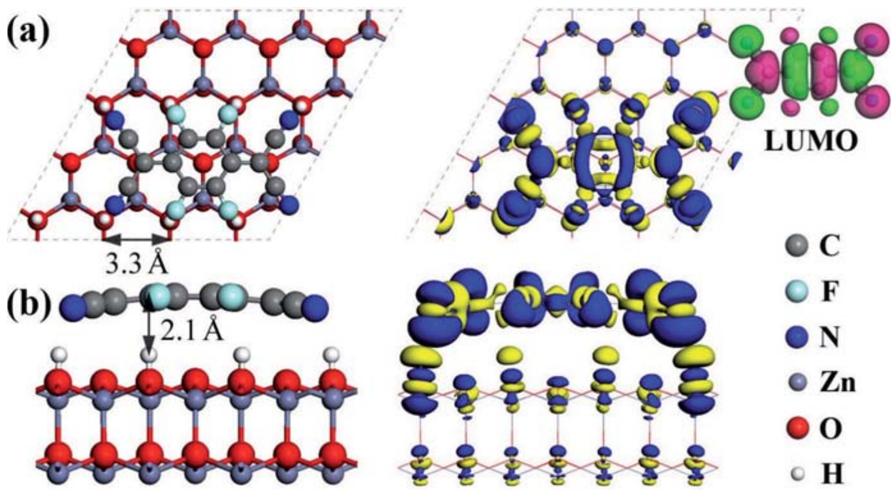
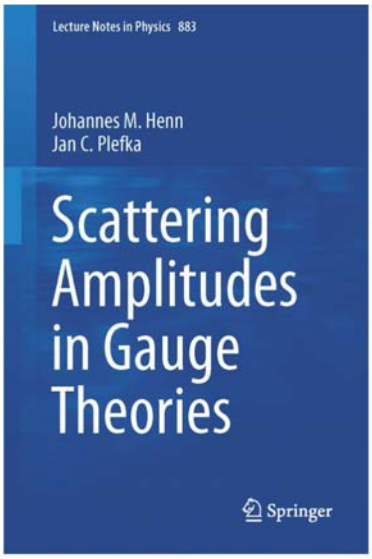


Fig. 2: Top (a) and side view (b) of F4TCNQ adsorbed on ZnO(000-1) (2 x 1)-H (left) and the adsorption-induced electron density rearrangement for n-doped ZnO (right). Electrons flow from the yellow to blue areas upon adsorption. The electron accumulation region mimics the shape of the lowest unoccupied molecular orbital (LUMO) of the free F4TCNQ molecule.

The associated work-function changes are large, which is in line with photoemission experiments on the same system.

Band-Bending in Organic Semiconductors: the Role of Alkali-Halide Interlayers
H. Wang, P. Amsalem, G. Heimel, I. Salzmann, N. Koch, and M. Oehzelt
Advanced Materials 26 (2014) 925
DOI: 10.1002/adma.201303467

4.1.7 Scattering Amplitudes in Gauge Theories – A New Lecture Notes in Physics Book by J. Henn and J. Plefka



At the fundamental level, the interactions of elementary particles are described by quantum gauge field theory. The quantitative implications of these interactions are captured by scattering amplitudes, traditionally computed using Feynman diagrams. In the past decade tremendous progress has been made in our understanding of and computational abilities with regard to scattering amplitudes in gauge theories, going beyond the traditional textbook approach. These advances build upon on-shell methods that focus on the analytic structure of the amplitudes, as well as on their recently discovered hidden symmetries. In fact, when expressed in suitable variables the amplitudes are much simpler than anticipated and hidden patterns emerge.

These modern methods are of increasing importance in phenomenological applications arising from the need for high-precision predictions for the experiments carried out at the Large Hadron Collider, as well as in foundational mathematical physics studies on the S-matrix in quantum field theory.

Bridging the gap between introductory courses on quantum field theory and state-of-the-art research, there has been a need for a focused text book on the subject. Recently IRIS member Prof. Jan Plefka together with his former postdoc Dr. Johannes Henn, now at the Institute for Advanced Studies in Princeton (USA), have published the first monographical text on this fundamental subject. The concise yet self-contained and course-tested lecture notes are well-suited for a one-semester graduate level course or as a self-study guide for anyone interested in fundamental aspects of quantum field theory and its applications.

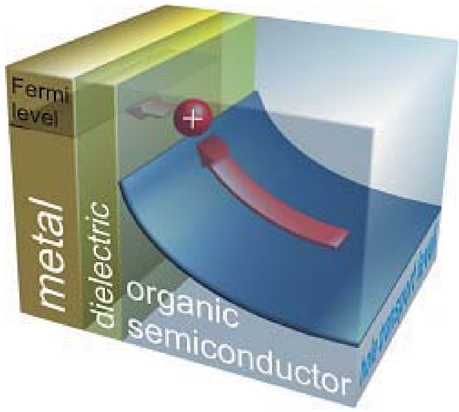
The book contains numerous exercises and solutions which help readers to embrace and apply the material presented in the main text.

Scattering Amplitudes in Gauge Theories
J. M. Henn and J. C. Plefka
Lecture Notes in Physics 883 (2014)
ISBN: 978-3-642-54021-9 (Print), 978-3-642-54022-6 (Online)

4.1.8 Energy-level Alignment at Metal/Organic Interfaces: Tying Up the Loose Ends

Organic semiconductors have tremendous potential for complementing conventional, inorganic semiconductors as active materials in (opto-)electronic devices such as light-emitting diodes (OLEDs) for display and lighting applications or solar cells (OPVCs). Electrical connection of such devices to peripheral circuitry, however, is realized by metallic contacts and the resulting interfaces to the organic semiconductor have played a central role: Energy barriers for injecting charge carriers into the organic (OLEDs) or energy losses upon their extraction (OPVCs) were found to detrimentally affect device performance. Attempts to minimize these energy barriers/losses have been hampered by an incomplete understanding of their origin and the parameters that govern their magnitude.

A multitude of sometimes conflicting views has been expressed in literature, each treating only a certain limiting case under particular assumptions for interface properties and dominant mechanism.



Schematic illustration of the electron transfer to acceptor states at a surface or interface of an n-doped semiconductor (middle and right). The development of a space-charge region induces band-bending, which brings the acceptor state closer to the Fermi level (right) In an undoped intrinsic semiconductor (left) no such electron transfer can take place resulting in an empty acceptor state in the band gap.

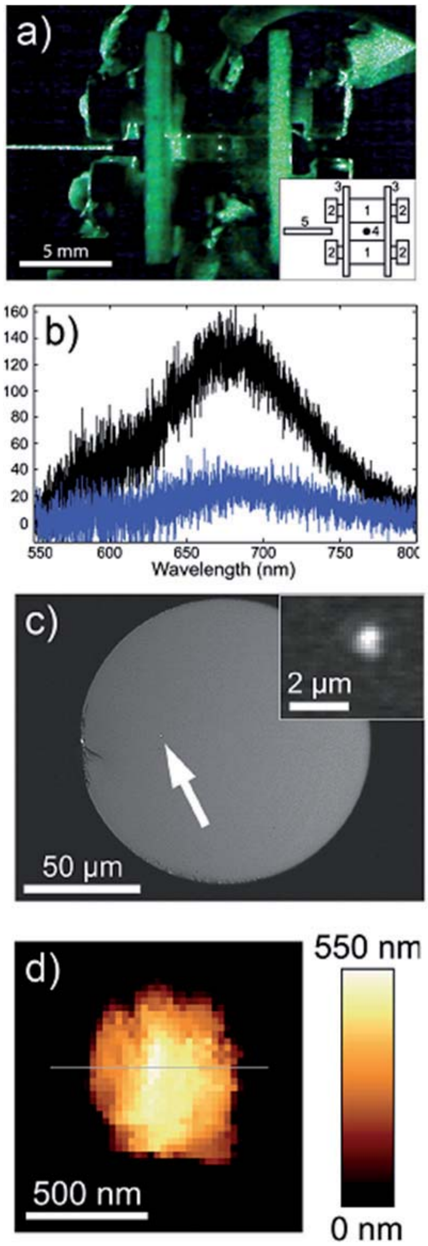
Now, a team, including IRIS-member Prof. Norbert Koch, implemented a detailed electrostatic model that can cover the full phenomenological range of interfacial energy-level alignment regimes within a single, consistent framework. Energy barriers/losses could be reproduced in both qualitative and quantitative agreement with a series of experiments. By continuously connecting the limiting cases described by previously proposed models, conflicting views in literature could be resolved. In particular, the team highlighted the key role played by the density of electronic states in the organic semiconductor: Its shape was found to determine both the minimum value of practically achievable injection barriers as well as their spatial profile, ranging from abrupt steps at the interface with the electrode to smoothly varying curves. Especially the latter – counter intuitively induced by introducing an ultrathin, electrically insulating interlayer between metal and organic – is beneficial for charge extraction in OPVCs, as illustrated below.

Organic semiconductor density of states controls the energy level alignment at electrode interfaces
M. Oehzelt, N. Koch, and G. Heimel
Nature Communications 5 (2014) 4174
DOI: 10.1038/ncomms5174

4.1.9 Defect Center Fluorescence from Levitated Diamonds

Researchers of the nanooptics group from the Department of Physics of the Humboldt-Universität zu Berlin have been able to levitate individual diamond particles while detecting the fluorescence emitted from the included defect centers. Prof. Oliver Benson, who is a member of **IRIS Adlershof**, and his group write in the scientific journal *Applied Physics Letters* how clusters of diamond nanoparticles have been stabilized in an electrodynamic trap, a so-called Paul trap. The used diamond clusters had diameters between some micro- and a few hundred nanometers and contained nitrogen vacancy (NV) defect centers. The defects were formed in the diamond lattice by a single nitrogen atom replacing a carbon atom with an adjacent lattice vacancy. Among the numerous known diamond defects, the

NV defects show remarkable optical and electronic properties, which make them ideal candidates for many different applications, e.g., as single photon emitters in quantum optics or markers in biological experiments.



The particles were charged and sprayed into the trap by electrospray ionization in order to confine them in the oscillating electric field. The researchers demonstrated how particle stability can be controlled by the trap parameters. The measured fluorescence emission spectra proved that the trapped particles were indeed diamonds with NV defects.

The size determination of the trapped particles occurred after optical characterization. The free levitated diamonds were deposited from the trap on the end faces of optical fibers. The clean and delimited area of a fiber face enabled easy retrieval of the particles. Subsequent measurements with optical and atomic force microscopes revealed that the smallest particles with detectable NV fluorescence had sizes of around 500 nm, so far. This means the collected fluorescence did not originate from one but several NV centers, a fact that could be already deduced from the fluorescence spectra.

The reason for this limitation can be found in the collection efficiency of the used microscope set up. The electrodes restricted the optical access to the trap center. For the next experiments, the researchers plan to involve improved trap geometries in order to detect the fluorescence emission of a single NV center in a single levitated diamond nanocrystal.

For an investigation of optomechanical interactions in single nanometer-sized diamond crystals, the spatial isolation of diamond clusters in combination with the observation of fluorescence emission is an important first step on the road to success.

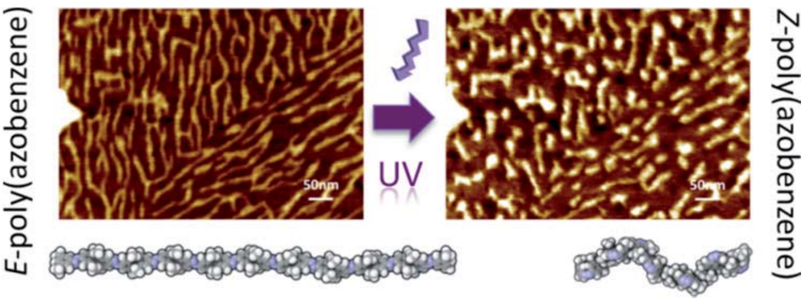
Nitrogen vacancy fluorescence from a submicron diamond cluster levitated in a linear quadrupole ion trap
A. Kuhlicke, A. W. Schell, J. Zoll, and O. Benson
Applied Physics Letters 105 (2014) 073101
DOI: 10.1063/1.4893575

4.1.10 Light-Induced Movements of Single Macromolecules on a Modified Graphite Surface

A current challenge to be addressed in nanotechnology is the ability to precisely control the motion of single molecules on an atomically well-defined surface, with the aim at developing "machines" that are able to perform actual work on the smallest scale. A common strategy consists in creating compounds so that external energy, either from chemical fuels or physical stimuli, converted into movement through concerted conformational changes. Physical stimuli like electrons or photons are particularly beneficial, as they offer a non-invasive, clean way of addressing molecules with very high spatial precision. Several works have already been reported on the electro- or photo-induced motion of relatively small molecules, which were typically observed with very-high resolution microscopes, such as scanning tunneling or atomic force microscopes (STM and AFM). These examples include small molecules resembling wheels, pinions, or even cars.

Although the level of complexity already reached with small molecules is quite impressive, longer molecules, such as polymers, are more promising for obtaining mechanical movements over larger distances.

As reported in *ACS Nano*, David Bléger, Jürgen P. Rabe, and coworkers, Chien-Li Lee, Tobias Liebig, and Stefan Hecht, from **IRIS Adlershof** and the Departments of Physics and Chemistry of the Humboldt-Universität zu Berlin have now realized a system, in which single polymers can be reversibly contracted and stretched onto a modified graphite surface by using two different types of light (UV and blue).



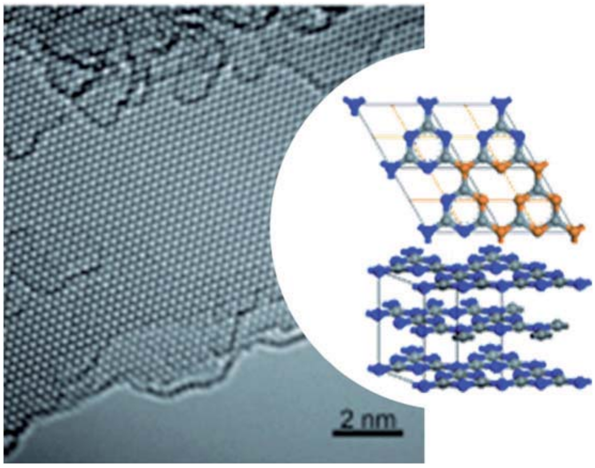
The macromolecules, which were visualized by AFM, were found to contract with large amplitudes and sometimes moved across the surface with what resembled a "crawling" movement. The key to achieving these motions was first to design polymers, in which dramatic contractions could be reversibly induced by light, and second to modify the surface by simultaneously orienting the linear macromolecules, isolating them from each other, and decoupling them from the surface. The next steps will consist of finding ways to control the directionality of the movements, thus opening up new possibilities for the development of optomechanical nanosystems.

Light-Induced Contraction and Extension of Single Macromolecules on a Modified Graphite Surface
C.-L. Lee, T. Liebig, S. Hecht, D. Bléger, and J.P. Rabe
ACS Nano 8 (2014) 11987
DOI: 10.1021/nn505325w

Featured in: Watching Single Molecules Move in Response to Light
P. K. Kundu and R. Klajn,
ACS Nano 8 (2014) 11913
DOI: *10.1021/nn506656r*

4.1.11 Long Sought Two-Dimensional Graphitic Semiconductor Discovered

A European team of chemists and physicists, including Dr. Nikolai Severin and Professor 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 theoretically predicted 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 have been known so far: graphene itself, hexagonal boron nitride, boron carbon nitride, fluorographene, and graphene oxide. TGCN is structurally similar to graphite but is a semiconductor, which is of high interest for opto-electronic applications. Cooperation partners in this project are Dr. Michael J. Bojdys and Professor Arne Thomas (TU Berlin), Professor 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 Optics and Electronics".



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
Angewandte Chemie Int. Ed., 53 (2014) 7450–7455
DOI: 10.1002/anie.201402191

4.2 Selected Publications

- Synthesis and properties of branched oligo(2-thienyl)- and oligo(2,2'bithien-5-yl)-substituted pyridine derivatives
  M. K. Bera, S.L. Gholap, P. Hommes, K. Neuthe, D. Trawny, J. P. Rabe, D. Lentz, R. Zimmer, and H.-U. Reissig
  Adv. Synth. Catal. 355 (2013) 3463, DOI: 10.1002/adsc.201300613

- Yangian symmetry of smooth Wilson loops in N=4 super Yang-Mills theory D. Müller, H. Münkler, J. Plefka, J. Pollok, and K. Zarembo
  J. High En. Phys. 2013 (2013) 81, DOI: 10.1007/JHEP11(2013)081

- Angles, Scales and Parametric Renormalization
  F. Brown and D. Kreimer
  Lett. Math. Phys.103 (2013) 933, DOI: 10.1007/s11005-013-0625-6
  link.springer.com/article/10.1007/s11005-013-0625-6

- Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100)
  N. A. Richter, S. Sicolo, S. V. Levchenko, J. Sauer, and M. Scheffler
  Phys. Rev. Lett. 111 (2013) 045502, DOI: 10.1103/PhysRevLett.111.045502

- Statistics of time-dependent rupture of single ds-DNA
  H. Liang, N. Severin, S. Fugmann, I. M. Sokolov, and J. P. Rabe
  J. Phys. Chem. B 117 (2013) 8875, DOI: 10.1021/jp400872k

- Influence of graphene exfoliation on the properties of water-containing adlayers visualized by graphenes and scanning force microscopy
  B. Rezania, M. Dorn, N. Severin, and J. P. Rabe
  J. Coll. Interf. Sci. 407 (2013) 500, DOI: 10.1016/j.jcis.2013.06.034

- The impact of edges and dopants on the work function of graphene nanostructures. The way to high electronic emission from pure carbon medium.
  D. G. Kvashnin, P. B. Sorokin, J. W. Brüning, and L. A. Chernozatonskii
  Appl. Phys. Let. 102 (2013) 183112, DOI: 10.1063/1.4804375

- Exfoliation of crystalline 2D carbon nitride: thin sheets, scrolls and bundles via mechanical and chemical routes.
  M. J. Bojdys, N. Severin, J .P. Rabe, A. Thomas, A. I. Cooper, and M. Antonietti
  Macromol. Rapid Commun. 34 (2013) 850, DOI: 10.1002/marc.201300086

- Splitting of lower energy levels in a quantum double well in a magnetic field and tunneling of wave packets in Nanowires
  J. Brüning, S. Yu. Dobrokhotov, and R. V. Nekrasov
  Theo. and Math. Phys.175 (2013) 620, DOI: 10.1007/s11232-013-0051-z

- Exploring the bonding of large hydrocarbons on noble metals: Diindoperylene on Cu(111), Ag(111), and Au(111)
  C. Bürker, N. Ferri, A. Tkatchenko, A. Gerlach, J. Niederhausen, T. Hosokai, S. Duhm, J. Zegenhagen, N. Koch, and F. Schreiber
  Phys. Rev. B 87 (2013) 165443, DOI: 10.1103/PhysRevB.87.165443

- Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor
  R. Schlesinger, Y. Xu, O. T. Hofmann, S. Winkler, J. Frisch, J. Niederhausen, A. Vollmer, S. Blumstengel, F. Henneberger, P. Rinke, M. Scheffler, and N. Koch
  Phys. Rev. B 87 (2013) 155311, DOI: 10.1103/PhysRevB.87.155311

- Valence band structure of rubrene single crystals at the contact with an organic gate dielectric
  Y. Nakayama, J. Niederhausen, S. Machida, Y. Uragami, H. Kinjo,
  A. Vollmer, J. P. Rabe, N. Koch, and H. Ishii
  Org. Electron. 14 (2013) 1825, DOI: 10.1016/j.orgel.2013.04.019

- Role of the effective mass and interfacial dipoles on exciton dissociation in organic donor-acceptor solar cells
  C. Schwarz, S. Tscheuschner, J. Frisch, S. Winkler, N. Koch, H. Bässler, and Anna Köhler
  Phys. Rev. B 87 (2013) 155205, DOI: 10.1103/PhysRevB.87.155205

- Three-dimensional quantum photonic elements based on single nitrogen vacancy-centres in laser-written microstructures
  A. W. Schell, J. Kaschke, J. Fischer, R. Henze, J. Wolters, M. Wegener, and O. Benson
  Sci. Rep. 3 (2013) 1577, DOI: 10.1038/srep01577

- On the gluing formula for the analytic torsion
  Jochen Brüning and Xiaonan Ma
  Math. Zeit. 273 (2013) 1085, DOI: 10.1007/s00209-012-1045-5

- Four-loop corrections with two closed fermion loops to fermion self energies and the lepton anomalous magnetic moment
  R. Lee, P. Marquard, A. V. Smirnov, V. A. Smirnov, and M. Steinhauser
  Jour. High En. Phys., 2013 (2013) 162, DOI: 10.1007/JHEP03(2013)162

- Origin of mechanical strain sensitivity of pentacene thin-film transistors
  V. Scenev, P. Cosseddu, A. Bonfiglio, I. Salzmann, N. Severin, M. Oehzelt, N. Koch, and J. P. Rabe
  Org. Electron. 14 (2013) 1323-1329, DOI: 10.1016/j.orgel.2013.02.030

- Moderate doping leads to high performance of semiconductor/insulator polymer blend transistors
  G. 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
  Nature Communications 4 (2013) 1588, DOI: 10.1038/ncomms2587

- Ultrafast two-dimensional terahertz spectroscopy of elementary excitations in solids
  M. Woerner, W. Kuehn, P. Bowlan, K. Reimann, and T. Elsaesser
  New J. Phys. 15 (2013) 025039, DOI: 10.1088/1367-2630/15/2/025039

- Charged and metallic molecular monolayers through surface-induced aromatic stabilization
  G. Heimel, S. Duhm, I. Salzmann, A. Gerlach, A. Strozecka, J. Niederhausen, C. Bürker, T. Hosokai, I. Fernandez-Torrente, G. Schulze, S. Winkler, A. Wilke, R. Schlesinger, J. Frisch, B. Bröker, A. Vollmer, B. Detlefs, J. Pflaum, S. Kera, K. J. Franke, N. Ueno, J. I. Pascual, F. Schreiber, and N. Koch
  Nature Chemistry 5 (2013) 187–194, DOI: 10.1038/nchem.1572

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

- Electronic structure of CoPc adsorbed on Ag(100): Evidence for molecule-substrate interaction mediated by Co 3d orbitals
  E. Salomon, P. Amsalem, N. Marom, M. Vondracek, L. Kronik, N. Koch, and T. Angot
  Phys. Rev. B 87 (2013) 075407, DOI: 10.1103/PhysRevB.87.075407

- Design and numerical optimization of an easy-to-fabricate photon-to-plasmon coupler for quantum plasmonics
  G. Kewes, A. W. Schell, R. Henze, R. S. Schönfeld, S. Burger, K. Busch, and O. Benson
  Appl. Phys. Lett. 102 (2013) 051104, DOI: 10.1063/1.4790824

- Comparing efficient computation methods for massless QCD tree amplitudes: Closed analytic formulas versus Berends-Giele recursion
  S. Badger, B. Biedermann, L. Hackl, J. Plefka, T. Schuster, and P. Uwer
  Phys. Rev. D 87 (2013) 034011, DOI: 10.1103/PhysRevD.87.034011

- Role of charge transfer, dipole-dipole interactions, and electrostatics in Fermi-level pinning at a molecular heterojunction on a metal surface
  P. Amsalem, J. Niederhausen, A. Wilke, G. Heimel, R. Schlesinger, S. Winkler, A. Vollmer, J. P. Rabe, and N. Koch
  Phys. Rev. B 87 (2013) 035440, DOI: 10.1103/PhysRevB.87.035440

- Electronic Structure of Individual Hybrid Colloid Particles Studied by Near-Edge X-ray Absorption Fine Structure (NEXAFS) Spectroscopy in the X-ray Microscope
  K. Henzler, P. Guttmann, Y. Lu, F. Polzer, G. Schneider, and M. Ballauff
  Nano Lett. 13 (2013) 824, DOI: 10.1021/nl3046798

- Measurement of the Ultrafast Spectral Diffusion of the Optical Transition of Nitrogen Vacancy Centers in Nano-Size Diamond Using Correlation Interferometry
  J. Wolters, N. Sadzak, A. W Schell, T. Schroeder, and O. Benson
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- Temperature independent tuning of whispering gallery modes in a cryogenic environment
  R. Henze, J. M. Ward, and O. Benson
  Opt Express 21 (2013) 675-680, DOI: 10.1364/OE.21.000675

- Modular Synthesis of Monomers for On-Surface Polymerization to Graphene Architectures
  M. Gille, A. Viertel, S. Weidner, and S. Hecht
  Synlett 24 (2013) 259-263, DOI: 10.1055/s-0032-1317959

- MR-search: massively parallel heuristic search
  T. Schütt, A. Reinefeld, and R. Maier
  Concurr. Comp.-Pract. E 25 (2013) 40-54, DOI: 10.1002/cpe.1833

- Thermophoresis of thermoresponsive polystyrene–poly(N-isopropylacrylamide) core–shell particles
  A. Königer , N. Plack , W. Köhler , M. Siebenbürger, and M. Ballauff
  Soft Matter 9 (2013) 1418-1421, DOI: 10.1039/C2SM27417E

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  D. Kreimer and A. Velenich
  Lett. Math. Phys. 103 (2013) 171–181, DOI: 10.1007/s11005-012-0589-y

- Switching with orthogonal stimuli: electrochemical ring-closure and photochemical ring-opening of bis(thiazolyl)maleimides
  M. Herder, M. Utecht, N. Manicke, L. Grubert, M. Pätzel, P. Saalfrank, and S. Hecht
  Chem. Sci. 4 (2013) 1028-1040, DOI: 10.1039/C2SC21681G

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  K. Akaike, N. Koch, and M. Oehzelt
  Appl. Phys. Lett. 105 (2014) 223303, DOI: 10.1063/1.4903360

- Charge transfer in and conductivity of molecularly doped thiophene-based copolymers
  F. Ghani, A. Opitz, P. Pingel, G. Heimel, I. Salzmann, J. Frisch, D. Neher, A. Tsami, U. Scherf, and N. Koch,
  J. Polym. Sci. B Polym. Phys. 53 (2014) 5, DOI: 10.1002/polb.23631

- Lattice Matching as the Determining Factor for Molecular Tilt and Multilayer Growth Mode of the Nanographene Hexa-*peri*-hexabenzocoronene
  P. Beyer, T. Breuer, S. Ndiaye, A. Zykov, A. Viertel, M. Gensler, J. P. Rabe, S. Hecht, G. Witte, and S. Kowarik
  ACS Appl. Mater. Interfaces 6 (2014) 21484, *DOI:* 10.1021/am506465b

- Single crystalline Er_2O_3:sapphire films as potentially high-gain amplifiers at telecommunication wavelength
  A. S. Kuznetsov, S. Sadofev, P. Schäfer, S. Kalusniak, and F. Henneberger
  Appl. Phys. Lett. 105 (2014) 19111, *DOI:* 10.1063/1.4901819

- Hydride Binding to the Active Site of [FeFe]-Hydrogenase
  P. Chernev, C. Lambertz, A. Bruenje, N. Leidel, K. Sigfridsson, R. Kositzki, C.-H. Hsieh, S. Yao, R. Schiwon, M. Driess, C. Limberg, T. Happe, and M. Haumann
  Inorg. Chem. 53 (2014) 12164, DOI: 10.1021/ic502047q

- Light-Induced Contraction and Extension of Single Macromolecules on a Modified Graphite Surface
  C.-L Lee, T. Liebig, S. Hecht, D. Bléger, and J. P. Rabe
  ACS Nano 8 (2014) 11987, DOI: 10.1021/nn505325w

  Featured in:
  Watching Single Molecules Move in Response to Light
  P. K. Kundu and R. Klajn
  ACS Nano 8 (2014) 11913, DOI: 10.1021/nn506656r

- In situ synthesis of semiconductor nanocrystals at the surface of tubular J-aggregates
  Y. Qiao, F. Polzer, H. Kirmse, E. Steeg, S. Kirstein, and J. P. Rabe
  J. Mater. Chem. C 2 (2014) 9141, DOI: 10.1039/C4TC01724B

- Green emission in ladder-type Quaterphenyl: Beyond the Fluorenone-defect
  B. Kobin, F. Bianchi, S. Halm, J. Leistner, S. Blumstengel, F. Henneberger, and S. Hecht
  Adv. Funct. Mater. 24 (2014) 7717, DOI: 10.1002/adfm.201402638

- Synthesis, Characterization and Interconversion of β-diketiminato Nickel N_xH_y Complexes
  C. Köthe, B. Braun, C. Herwig, and C. Limberg
  Eur. J. Inorg. Chem. 31 (2014) 5296, DOI: 10.1002/ejic.201402812

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  C. Draxl, D. Nabok, and K. Hannewald
  Acc. Chem. Res. 47 (2014) 3225, DOI: 10.1021/ar500096q

- Narrow-band single photon emission at room temperature based on a single nitrogen-vacancy center coupled to an all-fiber-cavity
  R. Albrecht, A. Bommer, C. Pauly, F. Mücklich, A.W. Schell, P. Engel, T. Schröder, O. Benson, J. Reichel, and C. Becher
  Appl. Phys. Lett. 105, (2014) 073113, DOI: 10.1063/1.4893612

- 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, and C. Draxl
  J. Phys.: Condens. Mat. 26 (2014) 363202, DOI: 10.1088/0953-8984/26/36/363202

- Nitrogen vacancy center fluorescence from a submicron diamond cluster levitated in a linear quadrupole ion trap
  A. Kuhlicke, A. W. Schell, J. Zoll, and O. Benson
  Appl. Phys. Lett. 105 (2014) 073101, DOI: 10.1063/1.4893575

- Harnessing the Liquid-Phase Exfoliation of Graphene Using Aliphatic Compounds: A Supramolecular Approach
  A. Ciesielski, S. Haar, M. El Gemayel, H. Yang, J. Clough, G. Melinte, M. Gobbi, E. Orgiu, M. V. Nardi, G. Ligorio, V. Palermo, N. Koch, O. Ersen, C. Casiraghi, and P. Samorì
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- A Cubic Fe_4Mo_4 Oxo Framework and Its Reversible Four-Electron Redox Chemistry
  J.P. Falkenhagen, B. Braun, E. Bill, D. Sattler, and C. Limberg
  Inorg. Chem. 53 (2014) 7294, DOI: 10.1021/ic500584a

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4.3 Scientific Conferences and Seminars

An important platform for communicating scientific results from **IRIS Adlershof** are 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.

Furthermore, **IRIS Adlershof** has organized the following scientific events, which **IRIS Adlershof** members substantially helped put together:

4.3.1 Hybrid-Photovoltaics 2013 Symposium

May 15-17, 2013

This symposium was organized by the Helmholtz-Energy-Alliance "Hybrid Photovoltaics" and focused on the following topics:

- Charge and energy transfer mechanisms at organic/inorganic hybrid interfaces
- Charge generation mechanisms at hybrid interfaces
- Photonic enhancement of charge generation
- Theoretical methods to describe electronic and optical excitations in hybrid materials
- Hybrid organic/inorganic photovoltaic devices: optimization and energy generation concepts.

4.3.2 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.

4.3.3 KOSMOS Summer University – Multiple Zeta Values in Mathematics and Physics

October 1-5, 2013

The KOSMOS Summer University "Multiple Zeta Values in Mathematics and Physics" investigated the role of multiple zeta values in algebraic and arithmetic geometry as well as in physics and furthermore studied the mutual interplay of these phenomena.

This five-day event primarily brought together graduated students and postdoctoral researchers in mathematics and theoretical physics with current leaders in their fields to vitalize scientific exchange and to give an understanding of current research questions.

The main aspects that were considered by the speakers:

- Multiple zeta values from algebraic geometry to physics
- Multiple zeta values, polylogarithms and elliptic curves
- From the structure of renormalizable quantum fields to periods of Feynman graphs
- Multiple zeta values and single-valued multiple polylogarithms
- Multiple zeta values and graph hypersurfaces
- Periods of hyperplane arrangements and their motivic Galois theory.

The home universities of our KOSMOS fellows, Prof. Francis Brown (CNRS, Paris) and Prof. José Burgos (ICMAT, Madrid), also agreed to participate as partner universities to continue this promising cooperative work.

One example for this collaboration was a supplementary summer school which took place at the ICMAT Madrid in December 2014.

4.3.4 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 light-weight devices with mechanical flexibility, e.g., in smart clothing. Yet another pressing challenge is the efficient generation of energy from renewable sources, such as photovoltaics, which needs to become available short-term in substantial quantity. Established materials have been pushed close to their intrinsic limits and many of the devices and systems using these materials are not light weight 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 opto-electronics 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 opto-electronic applications are at a comparably 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 opto-electronic 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.

4.3.5 Joint TAU –HU Workshop „Biological and Soft Matter Physics: Implications for Cell Biology, Nano-Bio-Technology and Medicine"

November 22-23, 2013

Biological physics and soft matter physics are emerging fields for the understanding of biological structures and processes. They allow development of materials that mimic biological structures which can be used in nano-biotechnology or for medical purposes, e.g., for regenerative therapies. The universities involved have complementing expertise in these fields, which provides an attractive basis for joint highly innovative projects. The aim of the proposed program is to create an interdisciplinary platform for both senior scientists and junior researchers of Humboldt-Universität zu Berlin and Tel Aviv University to collaborate on the physical principles governing the interdependent functioning of single biological molecules, their ensembles and aggregates, both in vitro and in living cells. Therefore a joint workshop to identify common areas of research took place in November 2013. At the end of the year, they called for proposals to be funded in a bilateral funding scheme. Funding is available for bilateral collaborative research projects comprising researchers or research teams from the two participating universities. The main goal of the program is to support the ongoing and stimulate new collaborations between the research groups of the two Universities.

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

July 8-19, 2014

The main objective of this KOSMOS Summer University was to teach fundamentals of the physics and chemistry of (opto-)electronic materials. The focus was on an integrative approach combining the key expertise from scientists representing the "three Ms": Make, Measure, and Model. Therefore, the event brought together young researchers from different backgrounds to generate a creative and interactive learning environment. The program was composed of tutorials and research highlights by current leaders in their field as well as critical analysis of the literature and the development of innovative ideas (proposals) in smaller interdisciplinary teams.

Thereby, the following topics were addressed:

- Electronic structure theory
- Synthesis of molecular materials
- Spectroscopic techniques
- Materials classes and properties
- Interfacial design and analysis
- Device fabrication and characterization

The program was complemented by various other activities involving the unique research and innovation environment of the science and technology park Berlin-Adlershof.

4.3.7 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 Prof. Klaus Müllen and Prof. 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.

5 Promotion of Young Scientists

IRIS members are involved in teaching classes at their corresponding departmental institutes. Especially with special lectures that go into detail about the IRIS research areas, it is thus possible to interest students in scientific work at **IRIS Adlershof** and to integrate master and doctoral students in **IRIS Adlershof** research projects. The first joint workshop with Princeton University in October 2013 was coupled with a Young Researchers Satellite workshop that was completely organized by early-stage researchers and open to interested early-stage researchers from master students on up to junior professors.

IRIS Adlershof has directly supported these young scientists in the report period. Four early-stage researchers were given start-up and interim funds that were financed by IRIS. IRIS also paid for guest stays at **IRIS Adlershof** for two further early-stage researchers.

A special effort was made by **IRIS Adlershof** to support the internationalization of young scientistics in two ways. First the recruitment of doctoral students and postdocs was directly used to increase the number of international early-stage researchers in IRIS research groups. This benefited, for example, the above-mentioned measures from start-up and interim funds and the guest stays of several applicants with international background. For one thing, this gave German doctoral students and post-docs more mobility, particularly, for guest research stays abroad. IRIS was thus able to promote international student exchange, especially by providing lab training to interested bachelor students from NUS and by integrating advanced master and doctoral students as well as postdocs in the early stages of current research cooperations with international partners.

Dr. Georg Heimel from Prof. Koch's group co-organized the symposium "Computational Modelling of Organic Semiconductors: From the Quantum World to Actual Devices" in the framework of the 2014 spring meeting of the European Materials Research Society (Lille, France, May 26-30, 2014. The event was financially supported by **IRIS Adlershof**.

The internationalization of young scientists also took place, particularly within appropriately structured programs like international research training groups and initial training networks. **IRIS Adlershof** also had an excellent record in this area in the report period.

In February 2014 **IRIS Adlershof** organized a series of seminars on scientific writing targeting to young researchers working on IRIS relevant research areas. The two-day seminars were held by a Canadian linguist who specializes in technical and engineering communication. The seminar focused on solving problems scientific writers face when they communicate their work in English. A series of linguistic principles for communicating research in the clearest, most coherent, convincing, and concise manner was presented.

IRIS Adlershof's young scientists had impressive and successful results in the report period. The Physical Society of Berlin awarded Dr. Tim Schröder the Carl-Ramsauer prize in

2013 for his doctoral thesis in the Benson research group, "Integrated Photonic Systems for Single Photon Generation and Quantum Applications: Assembly of Fluorescent Diamond Nanocrystals by Novel Nano-Manipulation Techniques". Dr. Konstantin Wiegandt was distinguished by the Humboldt Prize from our university for his dissertation, "Superconformal Quantum Field Theories in String - Gauge Theory Dualities", which he did in Prof. Plefka's group. Additionally, Janik Wolters from the Benson group won the Berlin Science Slam as well as the Carl-Ramsauer and Humboldt prizes for his dissertation on "Integrated Photonic Systems for Single Photon Generation and Quantum Applications: Assembly of Fluorescent Diamond Nanocrystals by Novel Nano-Manipulation Techniques". Phillip Lange from the Rabe group won the Lise-Meitner Prize in 2014 for the best dissertation. The title of his work was "Optical and Structural Properties of Systems of Conjugated Molecules and Graphenes".

Dr. Martin Hempel for Prof. Elsässer's group won the Adlerhof dissertation of the year prize for 2014 for his doctoral thesis on defective mechanisms in high-performance diode lasers.In the annual competition "Forum Junge Spitzenforscher" launched by the foundation Stiftung Industrieforschung in cooperation with the Humboldt-Innovation GmbH, Andreas Schell, who is a PhD student in the group of Prof. Oliver Benson, was awarded second prize for his contribution "Novel Hybrid Materials for Quantum Optical Applications". Mr. Schell was financially supported by **IRIS Adlershof**.

Matteo Guzzo was awarded with a Humboldt Research Fellowship for Postdoctoral Researchers by the Alexander von Humboldt Foundation. This is going to support the work in his new research area "Electron-Phonon Coupling in Photoemission Spectra within Advanced Greens Function Methods". Guzzo did a doctorate at the École Polytechnique, where his thesis on "Dynamical Correlations in Solids" was awarded the best dissertation in 2012. Since 2013 he has been working as a postdoc in Prof. Claudia Draxl's group on solid state theory and is also being funded by **IRIS Adlershof**.

Last but not least, Bita Rezania, who is a doctoral student in the graduate school SALSA and Prof. Rabe's group, was awarded the poster prize from the 2014 Adlershof Research Forum.

6 Honors and Awards

During the reporting period, IRIS members received the following awards and honors:

Prof. Dr. Jochen Brüning:

2013 Elected member of the Institute for Advanced Study Princeton, USA

Prof. Dr. Claudia Draxl:

2013 Caroline von Humboldt Professorship

2013 Paracelsusring of the city Villach

2014 Max Planck Fellow am Fritz-Haber-Institut Berlin

Prof. Dr. Norbert Koch:

2013 Visiting Professor at Chiba University, Japan

2014 Chair Professor of the Functional Nano & Soft Materials Laboratory (FUNSOM), Soochow University, China

Prof. Dr. Jürg Kramer:

2014 Elected member of the National Academy of Science and Engineering

Prof. Dr. Jan Plefka:

2014 Visiting Professor at the Institute of Theoretical Physics, ETH Zürich, Switzerland

Prof. Dr. Jürgen P. Rabe:

2014 Visiting Professor at Princeton University, USA

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