



Integrative Research Institute for the Sciences **Biannual Report 2015 & 2016**



Preface

Within its Institutional Strategy, funded through the framework of the German Excellence Initiative, Humboldt-Universität zu Berlin (HU) has set up Integrative Research Institutes (IRIs) that enable and promote top-level interdisciplinary research in fields, which are considered constitutional for HU's scientific profile. IRIs aim at connecting HU's outstanding core competences with its partners, including other universities, research institutes, and also industrial partners, in order to create an efficient institute for seminal interdisciplinary cooperation as well as to further the development of early career stage scientists.

The first IRI that HU founded in preparation of the last round of the Excellence Initiative was the Integrative Research Institute for the Sciences **IRIS Adlershof**, which 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".

An evaluation of IRIS, performed by an external expert commission in June 2016 has explicitly confirmed the successful development of **IRIS Adlershof** since its inception. The reviewers concluded, that IRIS has succeeded to put the HU's science campus, Berlin Adlershof on the international map of research in the fields of hybrid systems and mathematical physics.

Two years ago, we reported on the activities during the years 2013 and 2014. The present report reflects on the years 2015 and 2016. During this period IRIS has grown with three new members and an Emmy Noether Junior Research Group. Invited lectures at international conferences given by IRIS-members and scientific articles in reviewed journals regularly exceed the 100-peryear mark, documenting the high scientific output of IRIS's members. Among the highlights were the approval of a second funding period of the Collaborative Research Center (CRC) 951 "Hybrid Inorganic/Organic Systems for Optoelectronics" (HIOS) through the German Science Foundation (DFG), the successful finalization of the CRC 647 "Space-Time-Matter", as well as the successful application for funding of the EU-projects "Integrated self-assembled SWITCHable systems and materials: Towards responsive organic electronics – a multi-site innovative training action (iSwitch)" and "The novel materials discovery laboratory (NOMAD)".

Particularly important for the long run is the construction of the research building for the IRIS research area "Hybrid Systems for Optics and Electronics". The construction work started in February 2016 and the building should be ready for moving in and working in early of 2019.

It is my pleasure to thank all members and the staff of **IRIS** Adlershof for their dedicated work, and we are all very grateful for the wide range of the support that we have received from the administrative departments and the President's office of Humboldt-Universität zu Berlin.

Best wishes,

Jürgen P. Rabe, Chairman

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1. Introduction: The Integrative Research Institute for the Sciences

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 bridging 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".

Within the university IRIS is building new bridges in several respects:

- between the established disciplines chemistry, computer sciences, mathematics, and physics by specifically hiring bridging professors;
- between natural sciences, life sciences, humanities, and cultural sciences by close research and teaching collaboration with the IRI for Life Sciences and with the cluster of excellence "Image Knowledge Gestaltung";
- and between the university campuses Adlershof, Mitte, and Nord.

The establishment of **IRIS Adlershof** has led to closer cooperation between the various institutions involved. The most visible evidence of this is the appointment of joint professorships at the Departments of Physics and Chemistry or Physics and Mathematics, which are anchored in **IRIS Adlershof**. The active use of the spatial infrastructure of **IRIS Adlershof**, in particular the lecture rooms and the common rooms, has noticeably improved the contact between the disciplinary institutes. For example, the Graduate School SALSA has found a first "home" in the IRIS building and performs here regularly by events. At the same time, by encouraging close collaboration between research partners, **IRIS Adlershof** is a mean of exploiting potential at the interface of university and non-university research and of developing long-term collaborative research at Humboldt-Universität's natural science campus Adlershof.

1.1. Inner structure of IRIS Adlershof

IRIS Adlershof currently consists of 20 full members. In addition, four leaders of young researcher groups and about 140 early career researchers (graduate students, postdocs) have been associated with **IRIS Adlershof**.

IRIS Adlershof is headed by the IRIS Council, which currently consists of three members. The council decides on all important matters that are not in the competence of the general assembly or of other academic bodies. The council is headed by the chairman who represents IRIS internally and externally. The general assembly, as the highest body of **IRIS** Adlershof, is responsible for all decisions concerning the thematic, conceptual, and infrastructural development of **IRIS** Adlershof.

The chairman as well as the IRIS council is supported by a branch office that is responsible for all the administrative matters of **IRIS Adlershof**. The branch office relieves IRIS members of tasks outside the actual research, for example, by supporting the acquisition of third party funds, in the organization and conduct of scientific events, as well as in reports and general administrative issues.



Organization of IRIS Adlershof

Elected members of the IRIS-Council are:



Rabe, Jürgen P., Prof. Dr. (Chairman) Research Topic: Physics of macromolecules Humboldt-Universität zu Berlin, Department of Physics and Max Planck Institute for Colloids and Interfaces



Koch, Norbert, Prof. Dr. (Deputy Chairman)

Research Topic: Supramolecular Systems

Staudacher, Matthias, Prof. Dr.

Bridging Professorship Physics/Chemistry Humboldt-Universität zu Berlin, Department of Physics and Helmholtz-Zentrum Berlin für Materialien und Energie GmbH



Research Topic: Mathematical Physics of Space, Time and Matter Bridging Professorship Physics/Mathematics Humboldt-Universität zu Berlin, Department of Mathematics and Department of Physics

1.2. New members

IRIS has gained three new members during the reporting period:



List-Kratochvil, Emil, Prof. Dr. (IRIS-Member since 2015)

Research Topic: Hybrid Devices

Bridging Professorship Physics/Chemistry Humboldt-Universität zu Berlin, Department of Physics and Department of Chemistry

Emil List-Kratochvil, professor for Hybrid Devices at the Humboldt-Universität zu Berlin, joined **IRIS Adlershof** in November 2015. His position is a bridging professorship of **IRIS Adlershof** and it is embedded in both the departments of physics and chemistry of Humboldt-Universität

zu Berlin. Prof. List-Kratochvil is an leading expert on organic and printed electronics. He is internationally well known for his work on organic devices, as for instance light emitting diodes and hybrid storage elements.



Koch, Christoph T., Prof. Dr. (IRIS-Member since 2016) Research Topic: Structure Research and Electron Microscopy Humboldt-Universität zu Berlin, Department of Physics

Since November 2016 Christoph T. Koch, professor for structural research and electron microscopy at Humboldt-Universität's physics department and Nicola Pinna, professor for functional materials at the department of chemistry of Humboldt-Universität zu Berlin are new members at IRIS Adlershof. Christoph Koch's research focuses on the development of new methods in quantitative transmission electron microscopy (TEM) and their application to materials science problems.



Pinna, Nicola, Prof. Dr. (IRIS-Member since 2016) Research Topic: Functional Materials Humboldt-Universität zu Berlin, Department of Chemistry

Nanostructured materials are in the focus of Nicola Pinna's research interests. Special emphasis is laid on the synthesis of novel multifunctional materials, their characterization and the study of their physical properties.

Four young researcher groups are currently related to IRIS. The group leaders are:



Bléger, David, Dr.

Research Topic: Nanoscale and Photodynamic Systems Humboldt-Universität zu Berlin,

Department of Chemistry

David Bléger, who's position is funded by the German Research Foundation (DFG), has established the independent junior research group "Photodynamic Molecular systems and Materials". The research focuses on photoswitchable organic and inorganic materials as well as on single-molecule wires.



Forini, Valentina, Dr. Research Topic: Gauge Fields from Strings Humboldt-Universität zu Berlin, Department of Physics

Valentina Forini is the head of an independent junior research group funded by the Emmy Noether Programme of the DFG. Her research addresses current issues in the framework of the string/gauge correspondence, emphasizing their relation and qualitative reference to quantum chromodynamics as well as the "cross-fertilization" of established gauge-theoretical tools to strings and vice versa.



Lu, Yan, Dr.

Research Topic: Structure Analysis of Colloidal Particles Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

The research of the independent Helmholtz-Junior research group on colloid chemistry, headed by Yan Lu, mainly focuses on the design and fabrication of functional hybrid materials based on colloidal particles with versatile applications, such as catalysts, solar cells, and optical devices.



Ramelow, Sven, Dr.

Research Topic: Nonlinear Quantum Optics

Humboldt-Universität zu Berlin, Department of Physics

Since October 2016 Sven Ramelow is the head of the independent Emmy Noether research group Nonlinear Quantum Optics, which is associated to **IRIS Adlershof**. A main goal of his group is to pioneer and establish quantum imaging and spectroscopy in the technologically highly relevant mid-infrared wavelength regime.

1.3. Competences of IRIS Adlershof

IRIS Adlershof builds on the particular competences of Humboldt-Universität at its Campus Adlershof 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 the insight will be employed for novel applica-

tions 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 modelling on the other. With the rapid development of the architecture of high performance

computing, new dimensions of the extraction of quantitative information will be within reach. Additionally, more and more realistic images of reality will be created by using efficient algorithms.

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

1.4. Research Areas

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

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.

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 2015 and 2016, 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".

Remarkable highlights within the first named research area during the reporting period were the approval of a second funding period of the Collaborative Research Center (CRC) 951 "Hybrid Inorganic/ Organic Systems for Optoelectronics (HIOS)", as well as the successful application for funding of the EU-projects "Integrated self-assembled SWITCHable systems and materials: Towards responsive organic electronics – a multi-site innovative training action (iSwitch)" and "The novel materials discovery laboratory (NOMAD)". Other important collaborative projects are 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", which have been successfully accomplished in the end of 2015. Further coordinated joint projects were funded by various federal, state, and international funding institutions (see Chapter 3).

The second named IRIS-research area "Space-Time-Matter" has likewise developed very well. This is reflected by the very successful work of the CRC 647 "Space-Time- Matter: Analytic and Geometric Structures" and the EU-project "Gauge Theory as an Integrable system (GATIS)", which were accomplished at the end of the reporting period. Applications for follow-up projects are currently under preparation. Other highlights within this research area are the Research Training Group (RTG) 1504: "Mass, Spectrum, Symmetry: Particle Physics in the Era of the Large Hadron Collider" and the project "Gravitation and High Energy Physics", funded by the Einstein Foundation.

In total, the IRIS members have obtained extensive third-party funding in the report period. The amount managed by the Humboldt-Universität comes to 15.5 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 "Integrability in Gauge and String Theory" jointly held with the École Normale Supérieure Paris and the King's College London, took place at the Adlershof campus in August 2016. Further examples include cooperative projects with the Princeton University, the University of Singapore, and the Tel Aviv University.

IRIS Adlershof's start-up and interim funding allowed to support a number of excellent earlystage 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

In our last biennial report, we outlined how we could significantly improve **IRIS Adlershof**'s spatial infrastructure by completing the IRIS-building at "Zum Großen Windkanal 6".

When the IRIS building was finished, shortly before the current reporting period started, the conditions noticeably improved for the IRIS groups doing theoretical work. Other university institutions have also benefited from these improved conditions by taking advantage of our modern and well equipped seminar-, meeting-, child care-, and common rooms. The structural conditions of the IRIS building, however, did not allow highly specialized laboratories to be implemented in the same building.

That deficiency will be remedied by the construction of a new research building that is dedicated to the IRIS research area "Hybrid Systems for Optics and Electronics". For successful work in this research area 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. 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. This amount includes about 10 million euros for basic equipment inclusively largescale scientific instruments. The project supervisor, which is the Berlin's 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 building will house 2,500 square meters laboratories and 2,200 square meters of office space and common rooms. A main element of the new research building will be a group lab with standardized clean and grey room conditions. The construction work has started in February 2016 and the finished building complex should be ready for moving in and working in by the beginning of 2019.

IRIS Adlershof runs a core facility which provides laboratory infrastructure and equipment for its members and cooperation partners. 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 GmbH (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 supra-



Scanning electron microscope "Gemini SEM 500" for the new IRIS Research Building

molecular 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. The JLSR infrastructure was completed by purchasing a TERS (Tip-Enhanced Raman-Spectroscopy) microscope and a scanning electron 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-Institute, the Max-Born-Institute, the Paul-Drude-Institute, the Fraunhofer Institute for Applied Polymer Research, the Leibniz Institute for Crystal Growth (IKZ), and the Federal Institute for Materials Research and Testing (BAM).

HUMBOLDT ACCESS is a new concept for the promotion of the collaboration between IRIS Adlershof and pertinent scientific and industrial partners. Innovative high-tech enterprises and research institutes are invited to collaborate within HUMBOLDT ACCESS by sending their own personnel. HUMBOLDT ACCESS aims at the development and the implementation of tailored concepts for organic and molecular electronics. Based on an open lab concept, where IRIS-researchers, start-up companies, and industry partners work together in one lab, we have established HUMBOLDT ACCESS within IRIS to close the value-chain, by optimizing knowledge transfer between individuals with different focus. To foster knowledge and technology transfer, we support researchers in applications for pertinent state- and federal funding programs, and to find suitable company partners, as well as by providing adequate working resources. The Humboldt-Innovation GmbH supports HUMBOLDT ACCESS in management of inventions and patenting processes. We plan to pursue established and projected cooperations and to establish new cooperations with industry.

2.1.2. Institutional funding

IRIS Adlershof annually receives a basic financial support to cover its main office costs from the university's central funding. A further funding was allocated to **IRIS Adlershof** by Humboldt-Universität's institutional strategy that is being funded through the Excellence Initiative since November 2012.

2.2. Cooperation & Internationalization

IRIS Adlershof was developed for creating an excellent framework for cutting-edge research in natural sciences. It 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 promotes intra-university collaboration with a strong research focus and thus plays a decisive role in profile-building at the University, namely, in the natural sciences. As an interdisciplinary institute, IRIS is transversally positioned to Humboldt-Universität's disciplinary natural science departments of chemistry, computer sciences, mathematics, and physics as well as the department of cultural sciences. The interdisciplinarity is fostered through the cooperation with both the Faculty of Natural Sciences and the Central Institute Hermann von Helmholtz-Centre for Cultural Techniques. **IRIS** Adlershof reports directly to the president of Humboldt-Universität zu Berlin.



AEI	Max Planck Institute for Gravitational Physics (Albert Einstein Institute)
BAM	Bundesanstalt für Materialforschung und -prüfung
BASF	BASF - The Chemical Company
BMS	Berlin Mathematical School
Chiba U	Chiba University, Graduate School of Advanced Integration Science
CRC 647	Collaborative Research Center 647 Space - Time - Matter. Analytic and Geometric Structures
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
FU Berlin	Freie Universität Berlin
ні	Humboldt Innovation GmbH
HU ACCESS	Humboldt Access - Open Laboratory for Advanced Materials
HZB	Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
HZMO	Humboldt Center for Modern Optics
IAP	Fraunhofer Institute for Applied Polymer Research
IKG	Cluster of Excellence: Image Knowledge Gestaltung.An Interdisciplinary Laboratory
IKZ	Leibniz Institute for Crystall Growth
INAM	Innovation Network for Advanced Materials
Inuru	Inuru GmbH, Berlin
IRIS-LS	Integrative Research Institute of Life Sciences
JLSR	Joint Laboratory for Structural Research
КМРВ	Kolleg Mathematik Physik Berlin
LensWista	LensWista AG, Berlin
MATHEON	DFG-Research Center MATHEON
MBI	Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy
MPI-KG	Max Planck Institute of Colloids and Interfaces
MPI-P	Max Planck Institute for Polymer Research
Novaled	Novaled GmbH
NUS	National University of Singapore
PDI	Paul-Drude-Institut für Festkörperelektronik
PlasmaChem	PlasmaChem GmbH
Princeton	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	Universität Potsdam
WISTA	WISTA Management GmbH
ZIB	Zuse Institut Berlin

2.2.1. Innovation Network for Advanced Materials (INAM)



Intelligence, efficiency, and growing integrability: The rapid process in micro- and optoelectronics, optics and photonics, and the closely related material sciences defines the rate of further innovations and hence their effects on our prosperity and

innovation network for advanced materials

quality of life. Yet, the established silicon technology after decades of outstanding development is coming up against its limits. On the other hand, the transition to structured composite systems of various organic and inorganic materials on the nanolevel is revealing new properties and hence new prospects of applications in Adlershof thorough basic research is being conducted into these hybrid systems at **IRIS Adlershof** in close cooperation with numerous partners. With the view to accelerating the integration of these basic research findings in potential applications, scientists and science representatives came together to set up a new network.

In June 2016 the INAM Innovation Network for Advanced Materials e.V. was established following an initiative of the Science and Technology Park Berlin Adlershof. INAM spans the whole value chain from basic research to product design.

Next to industrial partners such as Osram GmbH, INAM's partners include the Integrative Research Institute for the Sciences (IRIS Adlershof), the Humboldt-Innovation GmbH, the economic development company Berlin Partner, and WISTA-MANAGEMENT GmbH. Initially planned for three years, the network's aim is to develop and implement concepts for the use of new materials and technology in electronics, optics, and photonics, which include, for example, new printing technology for cheaper production processes, transparent and conductive coatings for thin-film solar cells, or new organic light-emitting diodes (OLED) for the car industry.

The INAM network does more than to connect science and business and research and development. It also consists of partners who help to make products ready for the market. They range from the Pilotfish GmbH, a specialist for product design, to Fab Lab Berlin, an open workshop for development, or Humboldt Innovation GmbH and the attorneys of Weitnauer Rechtsanwälte Partnerschaftsgesellschaft, who offer advisory services on patents and technology transfer.

As their first big internationally visible activity, INAM has organized the Advanced Materials Competition (AdMaCom), which was a six-week workshop during August 28 to October 10, 2016 for developing innovative product concepts with international start-ups (see Chapter 4).

2.2.2. International Profile and Cooperations

One of IRIS Adlershof's overarching goals is to increase its international visibility in the two current IRIS-research areas "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter" and to profile the Adlershof campus as a place of international cutting-edge research. An important way to achieve this goal is to initiate new and intensify existing collaborations with international partner institutions. For this purpose we aim to further develop the cooperation with international partner institutions that are world leaders in the research areas "Hybrid Systems for Optics and Electronics" and "Space-Time-Matter". 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.

A joint research effort with researchers from Princeton University has been established, aimed at studying the fundamental chemical, electronic, and photonic interactions in novel opto-electronic materials and their combinations, and at developing new device types and architectures, including addressing manufacturing issues.



With the KOSMOS Summer Universities, Humboldt-Universität is bringing its international partnerships more closely into line with its high-profile research areas. In doing so, HU is focusing its international collaboration on excellent research partners and is making its research profile more visible around the world.

In 2016 Prof. Jan Plefka and Prof. Matthias Staudacher chaired a KOMSOS Summer University at Humboldt-Universität on "Integrability in Gauge and String Theory" (see Chapter 4). Prof. Vladimir Kazakov from LPT Ecole Normale Supérieure Paris and Prof. Nikolay Gromov from the King's College London spent an extended visit as KOSMOS Fellows at IRIS Adlershof. Prof. Nima Arkani-Hamed, one of the leading theoretical physicist of his generation, gave a public lecture on "Physics and Mathematics for the End of Spacetime".

The Ambassador of the People's Republic of China, Shi Mingde, visited the Science and Technology Park Adlershof, on April 8th, 2016 in the "Year of innovation cooperation between



Germany and China". At **IRIS Adlershof**, Founding Chairman Jürgen P. Rabe informed him on the research and development at IRIS on site in Adlershof as well as on cooperations with Chinese partners such as Beijing University and the Chinese Academy of Sciences. Shi Mingde was particular interested in the education of young scientists such as within the Berlin-wide Master Program on "Polymer Science", which has produced many, now internationally successful Chinese alumnae. The dialogue with Ambassador Shi Mingde, as begun here, shall be carried on.

3. Coordinated collaborative projects with participating IRIS members

3.1. IRIS Adlershof in the Excellence Initiative

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



(Period of funding 11/2012-10/2017) Spokespersons: Prof. Dr. Horst Bredekamp and Prof. Dr. Wolfgang Schäffner (both HU Berlin) 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

Cluster of Excellence "Unifying Concepts in Catalysis - UniCat"



(Period of funding 11/2007-10/2017) Spokesperson: 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. Nicola Pinna
- Prof. Dr. Joachim Sauer

Berlin Mathematical School



(Period of funding 11/2007-10/2017) Spokesperson: Prof. Dr. Jürg Kramer (IRIS Adlershof) (until 06/2016) Prof. Dr. Günther M. Ziegler (FU Berlin) (since 07/2016) 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

SCHOOL OF ANALYTICAL SCIENCES ADLERSHOF SALSA



measure is to know (Period of funding 11/2012-10/2017) Spokespersons: Prof. Dr. Janina Kneipp (HU Berlin) and Prof. Dr. Ulrich Panne (Federal Institute for Materials Research and Testing & HU Berlin) 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)

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



(Period of funding: 01/2005 – 12/2016) Spokesperson: Prof. Dr. Matthias Staudacher (IRIS Adlershof) 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
- Dr. Valentina Forini
- Prof. Dr. Dirk Kreimer
- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

CRC 658 "Elementary Processes in Molecular Switches at Surfaces"



(Period of funding: 07/2005 – 06/2017) Spokesperson: Prof. Dr. Martin Weinelt (FU Berlin) www.physik.fu-berlin.de/einrichtungen/sfb/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 interaction 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. Stefan Hecht, Ph.D.

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



(Period of funding: 01/2008 – 12/2019) Spokesperson: 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. Dr. Claudia Draxl
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Jürgen P. Rabe

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

Halbleiter-Nanopheconik SFB 787 (Period of funding: 01/2008 – 12/2019) Spokesperson: Prof. Dr. Michael Kneissl (TU Berlin) www.sfb787.tu-berlin.de

The CRC 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 multiterabus 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 Analysis and Stochastic, and the Konrad-Zuse-Zentrum für Informationstechnik.

Participating IRIS member:

• Prof. Dr. Oliver Benson

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



(Period of funding: 07/2011 – 06/2019) Spokesperson: Prof. Dr. Norbert Koch (IRIS Adlershof) www.physik.hu-berlin.de/sfb951

The CRC 951 is a central part of the IRIS research area "Hybrid Systems for Optics and Electronics". Here the scientists perform cutting-edge research on hybrid systems that unite inorganic semiconductors, metal nanostructures, and conjugated organic materials, with the aim to realize and tailor novel opto-electronic functions. The achievements made during the first funding period (2011-2015) laid the foundations for the next four years of exciting HIOS-research. In the long term, the CRC aims for solid-state opto-electronic devices that exhibit superior performance compared to those based on any of the individual material classes alone. The CRC's coordinator and vice-coordinator, Norbert Koch and Oliver Benson (both members of IRIS Adlershof), are delighted with the success in obtaining continued funding from the Deutsche Forschungsgemeinschaft (DFG), and they look forward to the joint work of 25 principal investigators from physics and chemistry of Humboldt-Universität zu Berlin (coordinating university), Technische Universität Berlin, Universität Potsdam, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, and Fritz-Haber-Institut der Max-Planck-Gesellschaft.

Participating IRIS members:

- Prof. Dr. Matthias Ballauff
- Prof. Dr. Oliver Benson
- Prof. Dr. Claudia Draxl
- Prof. Dr. Thomas Elsässer (until 06/2015)
- Prof. Stefan Hecht, Ph.D.
- Prof. Dr. Christoph Koch
- Prof. Dr. Norbert Koch
- Dr. Yan Lu
- Prof. Dr. Jürgen P. Rabe

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



(Period of funding: 04/2014 – 12/2017) Spokesperson: Prof. Dr. Christian Limberg (IRIS Adlershof) 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. Nicola Pinna
- Prof. Dr. Joachim Sauer

3.3. EU Research Projects

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:

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

iSwitch

"integrated self-assembled Switchable systems and materials: towards responsive organic electronics"



(Period of funding: 01/2015 - 12/2018) Coordinator: Prof. Paolo Samori (Université de Strasbourg) iswitch.u-strasbg.fr/index.php

iSwitch is a Marie Skłodowska-Curie Action Innovative Training Network (ITN) funded by the EU Framework Programme for Research and Innovation Horizon 2020. It offers top-level multi-disciplinary and supra-

sectorial training to a pool of talented young researchers, involving contributions from different scientific and technological fields such as, supramolecular chemistry, materials, nanoscience, physics and engineering. iSwitch's appointees will be trained through lecture courses, dedicated international schools and workshops, topical conferences, secondments to other consortium nodes and an ambitious and carefully planned research activities benefiting from the expertise of world-leading senior PIs and of younger but well-established PIs with outstanding track records in training and research. Additionally, iSwitch will generate new ground-breaking S&T knowledge needed to obtain efficient and fast switching in supramolecular electro- and opto-active materials as a response to external stimuli. This will be accomplished via controlled self-assembly of multicomponent architectures incorporating molecular switches, for fabricating responsive and multifunctional optoelectronic supramolecular devices. Special emphasis is laid on developing nano- and macro-scale switchable transistors and light-emitting devices as new solutions to (nanoscale) multifunctional organic-based logics.

Participating IRIS members:

- Prof. Stefan Hecht, PhD
- Prof. Dr. Norbert Koch

NOMAD

"The Novel Materials Discovery Laboratory"



(Period of funding: 11/2015 - 11/2018) Coordinator: Prof. Dr. Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft) http://nomad-coe.eu/

The NOMAD Laboratory is a European Centre of Excellence (CoE), funded by the European Union under the Horizon2020 program. Eight complementary research groups of highest

scientific standing in computational materials science along with four high-performance computing (HPC) centers form the synergetic core of this CoE.

New technological developments are practically always based on better, and often enough completely new, materials. This applies to the next generation of smartphones, fuel-efficient cars or powerful batteries for electric vehicles, as well as to catalysts for the production of methane or liquid fuels and high-performance solar cells. The NOMAD Laboratory develops a Materials Encyclopedia and Big-Data Analytics tools for materials science and engineering. It starts from the NOMAD Repository which contains data and input and output files of many high-quality calculations performed all over the word. The NOMAD Repository is unique in the sense that it is not restricted to one or a few simulation programs ("codes") but it accepts output from all important codes. In spring 2016 the NOMAD Repository contained input and output files of more than 2 million calculations which corresponds to more than 2 billion CPU-core hours burned on various high-performance computers all over the planet.

A Materials Encyclopedia will open up new opportunities by developing new tools to search and retrieve information from the large materials data pool. It will comprehensively characterize materials by their computed properties. The developed search engine enables to retrieve those materials that exhibit one or more required features.

Participating IRIS members:

- Prof. Dr. Claudia Draxl
- Prof. Johann-Christoph Freytag, Ph.D.

3.4. Research Training Groups and Graduate Schools

Research Training Group 1504 "Mass, Spectrum, Symmetry -Particle Physics in the Era of the Large Hadron Collider"



(Period of funding: 04/2009 - 03/2018) Spokesperson: Prof. Dr. Heiko Lacker (HU Berlin) 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 Universität zu Berlin and the Technische Universität 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:

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

International Research Training Group 1524 "Self-Assembled Soft Matter Nano-Structures at Interfaces"



(Period of funding: 04/2009-04/2018) Spokesperson: Prof. Dr. Martin Schoen (TU Berlin) www.ssni.tu-berlin.de

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 fieldinduced pattern formation of colloidal particles at interfaces.

Participating IRIS members:

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

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"

SOAMEDI

(Period of funding: 04/2010-09/2019) Spokesperson: Prof. Dr. Ulf Leser (HU Berlin) www.informatik.hu-berlin.de/en/forschung-en/gebiete/soamed-en

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.

International Research Training Group 1800 "Moduli and Automorphic Forms: Arithmetic and Geometric Aspects"



(Period of funding: 07/2012-12/2016) Spokesperson: Prof. Dr. Jürg Kramer (IRIS Adlershof) www.mathematik.hu-berlin.de/~grk1800

The international research training group (IRTG) aims at bundling the broad expertise in graduate education at HU Berlin / FU Berlin and at U Amsterdam / U Leiden in the field of arithmetic algebraic and complex algebraic geometry. More specifically, 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

International Max Planck Research School "Functional Interfaces in Physics and Chemistry"



Spokesperson: 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

International Max Planck Research School "Multiscale Bio Systems"



Spokesperson: 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

International Max-Planck Research School

"Mathematical and Physical Aspects of Gravitation, Cosmology and Quantum Field Theory"



(Period of funding: 01/2016-12/2027) Spokesperson: Prof. Dr. Hermann Nicolai (Max Planck Institute for Gravitational Physics) imprs-gcq.aei.mpg.de/2505/de

The International Max Planck Research School (IMPRS) for Mathematical and Physical Aspects of Gravitation, Cosmology and Quantum Field Theory addresses fundamental questions about the nature of classical and quantum gravity and its links to the fundamental constituents of matter. The research is purely theoretical and brings together some of the most exciting challenges of modern physics and mathematics. The school started operating in January 2016 and replaces the previous IMPRS for Geometric Analysis, Gravitation and String Theory.

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:

- Dr. Valentina Forini
- Prof. Dr. Dirk Kreimer
- Prof. Dr. Jan Plefka
- Prof. Dr. Matthias Staudacher

Graduate School Hybrid4Energy "Hybrid Materials for Efficient Energy Generation and Information Technologies"



(Funding since 04/2014) Spokesperson: Prof. Dr. Norbert Koch (IRIS Adlershof) 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. Norbert Koch
- Dr. Yan Lu
- Prof. Dr. Jürgen P. Rabe

GRADUATE SCHOOL PROMINTION

(Period of funding: 11/2014-10/2017) Spokespersons: Prof. Dr. Annette Upmeier zu Belzen & Prof. Dr. Burkhard Priemer (both HU Berlin) 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 member:

• Prof. Dr. Jürg Kramer

MASTER PROGRAM POLYMER SCIENCE



Head of Joint Commission: Prof. Dr. Reinhard Schömacker (TU Berlin) http://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 e.V.) became aware of this misbalance and initiated a two-year Master of Science polymer program, which started in the winter semester of 1999/2000. It was jointly designed by polymer scientists of the three Berlin universities, Freie Universität Berlin (FU), Humboldt-Universität Berlin (HU), Technische Universität Berlin (TU) and the nearby University of Potsdam (UP) with the goal in mind to be competitive with renowned polymer centers abroad. To make it more attractive to foreign students the program is in English.

This challenging interdisciplinary program benefits 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 work shops, 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 (Deputy Head of Joint Commission)

MASTER PROGRAM OPTICAL SCIENCES

Coordinator: Prof. Dr. Kurt Busch (HU Berlin) opticalsciences.physik.hu-berlin.de

The Optical Sciences comprise the study of the propagation and detection of light and its interaction with matter. Discoveries in optics have had a profound influence on the development of modern science and the forefront of technology, as demonstrated by more than 20 opticsrelated Nobel prizes between 1907 and 2014.

With the international MSc in Optical Sciences program, the Humboldt-Universität zu Berlin, together with its cooperation partners in the Science- and Technology-Park Berlin-Adlershof, offers an excellent education in this vibrant and exciting field.

Participating IRIS members:

- Prof. Dr. Oliver Benson
- Prof. Dr. Thomas Elsässer

3.5. Funding by the Einstein Foundation Berlin

ETERNAL

"Exploring Thermoelectric Propoerties of Novel Materials"



(Period of funding: 01/2013 – 03/2016) Spokesperson: Prof. Dr. Klaus-Robert Müller (TU Berlin) www.einsteinfoundation.de/personen-projekte/ einstein-forschungsvorhaben/

ETERNAL sets out to develop numerical tools to predict and analyze novel thermoelectric materials by linking theoretical physics, computational materials science, and machine learning. To achieve this ambitious goal, an innovative theoretical framework of new concepts and methods to describe, analyze, and understand materials and their functions will be developed. ETERNAL will systematically interweave density-functional theory, quantum chemistry, statistical mechanics, and machine learning.

Participating IRIS member:

• Prof. Dr. Claudia Draxl

"GRAVITATION AND HIGH ENERGY PHYSICS"



(Period of funding: 01/2013 – 01/2016) Spokesperson: Prof. Dr. Matthias Staudacher (IRIS Adlershof) www.einsteinfoundation.de/personen-projekte/ einstein-forschungsvorhaben/

A collaboration project funded by the Einstein Foundation Berlin between our working group at HU Berlin (Prof. Matthias Staudacher), the Albert Einstein Institute, Max Planck Institute for Gravitational Physics (Prof. Hermann Nicolai) and Hebrew University, Jerusalem (Prof Barak Kol). At all three locations, researchers are involved in the bridge between the theory of gravitation and the standard model of elementary particles, formulated as a quantum field theory. The project focuses on the exchange between different scientific approaches. While in Berlin modern methods of field theory, integrability and the calculation of scattering amplitudes are at the center, the Israeli partners are concerned with the effective field theory approach. Within the scope of binational workshops an intensive exchange and interest-sharing takes place.

Participating IRIS member:

• Prof. Dr. Matthias Staudacher

ACTIPLANT "Active Plasmonic nano-Antennas"



(Period of funding: 01/2014 – 01/2017) Spokesperson: Prof. Dr. Oliver Benson (IRIS Adlershof) www.einsteinfoundation.de/personen-projekte/ einstein-forschungsvorhaben/

The "Active Plasmonic nano-Antennas" (ActiPlAnt) – project, funded by the EINSTEIN Foundation, was launched in 2014. The main goals are the design, fabrication, testing and optimization of new types of structures to control the absorption and emission of photons by quantum emitters. Within this project the expertises in design, simulation, manufacturing, characterization and functionalization of nano structures and emitters of research groups form Humboldt-Universität and Hebrew University are combined.

Participating IRIS member:

Prof. Dr. Oliver Benson

ЕСМатн

"Einstein Center for Mathematics Berlin"



⊕ **EC**Math (Funding since 01/2014) Spokesperson: Prof. Dr. Michael Hintermüller (HU Berlin) www.ecmath.de/

The Einstein Center for Mathematics Berlin (ECMath) was founded in 2014. It is supported by the Einstein Foundation Berlin, by the three universities Freie Universität Berlin (FUB), Humboldt-Universität zu Berlin (HU), and Technische Universität Berlin (TUB) and by the two research institutes Weierstraß Institute for Applied Analysis and Stochastic (WIAS) and Zuse Institute Berlin (ZIB).

The main goals of ECMath are to support mathematical research in selected innovation areas and to establish and strengthen a network structure of excellent joint initiatives in Berlin.

Presently, ECMath includes, as founding members, the Research Center Matheon the Berlin Mathematical School (BMS) and the German Center for Teacher Education in Mathematics (DZLM) and as additional members the Research Campus Modal, the DFG Collaborative Research Centers (CRCs) 647, 1114, and Transregional Research Centers (TRs) 109, 154.

Through its versatile activities, ECMath aims at providing support for application-oriented basic research within Matheon, thus, targeting mathematics for innovation in key applications. By the conception of "Mathematics as a Whole", it fosters a comprehensive approach to mathematics and its applications through the training of young scientists and early-career students. Within this activity, ECMath provides attractive stipends for extraordinarily well-qualified BMS students, and it furthers and supports school activities of the DZLM. Another focus of ECMath is knowledge transfer from science to industry.

In this way, ECMath supports and creates an environment for connecting comprehensive mathematical education, cutting-edge research in pure and applied mathematics, and large-scale applications in industry and society.

Participating IRIS member:

• Prof. Dr. Jürg Kramer (member of the Executive Board)

3.6. More coordinated collaborative projects

Helmholtz-Energy-Alliance

"Inorganic / Organic Hybrid Solar Cells and Techniques for the Photovoltaics"



(Period of funding: 05/2012-12/2015) Spokesperson: Prof. Dr. Norbert Koch (IRIS Adlershof) http://www.helmholtz-berlin.de/pubbin/news_seite?nid=13471

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.

The aim of this energy alliance called "Inorganic / organic hybrid solar cells and techniques for photovoltaics" is to meet the urgent need for research to 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.

In the focus of research are processes that limit until 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, the researchers use among others nanostructures. So are inorganic nanoparticles and nanowires are placed in organic materials, wherein at the same time the cost effective production of such synthetic methods will be ensured. Very promising is also the embedding of organic semiconductor between inorganic nanorods.

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, 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 linked on the one hand virtually the activities of the partners and on

the other hand gets a real physical home at the Science and Technology Park Berlin-Adlershof. The Berlin Centre of Competence Thin Film and Nanotechnology for Photovoltaics, PVcomB, is associated as another partner.

Participating IRIS members:

- Prof. Dr. Claudia Draxl
- Prof. Stephan Hecht, PhD
- Prof. Dr. Norbert Koch
- Prof. Dr. Jürgen P. Rabe

3.7. 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 labour 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.

Humboldt-ProMINT-Kolleg

(Period of funding: 08/2010-03/2018) Spokesperson: Prof. Dr. Burkhard Priemer and Prof. Dr. Annette Upmeier zu Belzen (HU Berlin) www.promint.hu-berlin.de

The Humboldt-ProMINT-Kolleg is an interdisciplinary institution established at Humboldt-Universität zu Berlin cooperating 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. In this way the necessary requirements for an excellent and practice-oriented teacher education for the prospective candidates of the Master of Education are provided with a sustainable long-term effect.

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

Participating IRIS member:

• Prof. Dr. Jürg Kramer (Deputy Spokesman)

GERMAN CENTER FOR TEACHER EDUCATION IN MATHEMATICS (DZLM)



(Period of funding: 10/2011-12/2019) Director: Prof. Dr. Jürg Kramer (IRIS Adlershof) www.dzlm.de

The aim of the Deutsche Zentrum für Lehrerbildung Mathematik (DZLM) is the sustained improvement of the the mathematics teacher education in Germany. A consortium of six German universities coordinated by the Humboldt-Universität won the competetion 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 level, who teach outside of their expertise / 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 is including the Freie Universität Berlin, the Deutsche Universität für Weiterbildung in Berlin, the Ruhr-Universität Bochum, the Universität Duisburg-Essen and the Paderborn University. The concept of the university consortium provides, among other things, to build an online platform that informs mathematics teachers and teacher trainers on current developments in research and teaching and 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 peerreviewed 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

Doped organic semiconductors explored

Current semiconductor technology is based on silicon, an inorganic semiconductor material in which impurity atoms are introduced – or "doped" – for use in electronic components

to increase conductivity and tailor the electronic structure. However, organic solid-state materials made of conjugated molecules or polymers can also exhibit promising semiconducting properties that make their application feasible for organic electronics.

Guest molecules in a host structure

The enormous application potential of organic electronics has been clearly demonstrated for example by the success of organic LEDs (OLEDs) in the recent years. Oligothiophene (4T) and polythiophene (P3HT), two typical organic



x-ray diffraction on pure 4T. Credit: HZB

semiconductors, can be doped with a second type of molecule – such as a strong electron acceptor (F4TCNQ) for example – to control the electrical conductivity. However, until recently, how these guest molecules are exactly integrated into the host structure was poorly understood. A homogenous distribution analogous to that in inorganic semiconductors had therefore always been assumed.

Unusual characteristics

An international group headed by the Molecular Systems Joint Research Team at the HZB and Humboldt-Universität zu Berlin has now been able to demonstrate that this is not the case for either oligothiophene or polythiophene. The group, co-led by Dr. Ingo Salzmann and Prof. Norbert Koch, Deputy Chairman of IRIS Adlershof, had previously experimented with and already modelled other systems to learn how doping organic semiconductors affects their electronic structure and thus their conductivity. This produced clues about unusual characteristics of this class of materials in which hybridisation of the molecular orbitals plays a key role.

They therefore fabricated a series of organic thin films with increasingly heavy levels of doping and investigated these samples using X-ray diffraction techniques at the KMC-2 beamline managed by Dr. Daniel Többens. They were able to precisely determine the dependence of the crystalline structure on the degree of doping using this technique.

Co-crystallites as dopants

Their results for the organic semiconductors 4T and P3HT showed that the guest molecules – quite contrary to the expectations – are not uniformly incorporated in the host lattice at all. Instead, a second crystalline phase of host/guest co-crystallites is formed in the pure crystal-line host matrix. These co-crystals function in the role of dopant in place of the actual, pure doping molecules in such systems.

Better understanding for more control

"It is important to understand the fundamental processes involved in the molecular electrical doping of organic semiconductors more precisely", explains Salzmann, continuing: "If we want to successfully employ these kinds of materials in applications, we need to be able to control their electronic properties just as precisely as we customarily do today with inorganic semiconductors."

Charge-transfer crystallites as molecular electrical dopants

H. Méndez, G. Heimel, S. Winkler, J. Frisch, A. Opitz, K. Sauer, B. Wegner, M. Oehzelt, C. Röthel, S. Duhm, D. Többens, N. Koch and I. Salzmann *Nature Communications 6 (2015) 8560* DOI: 10.1038/ncomms9560

Flexible nanowires: A Berlin-Graz research team develops molecular wires with higher conductivity and bendability

The miniaturization of electronic building blocks has been relentlessly advancing for five decades. Meanwhile little "smart" cell phones have more computing power than entire computer centers from the early days. Each electronic device basically controls the charge current with transistors and circuit boards. Ultimately molecular switches and wires (molecular electronics) will reduce the size of these objects even further, but there still has to be high conductivity to ensure the electrical contact between the individual molecules. Furthermore, they should be bendable enough to adapt to flexible bases. The approaches followed so far have greater conductivity because of the stiffer wire structures, which are inherently rigid with a resultant lack of flexibility. Stefan Hecht's group has introduced an alternative approach in their recent work. In cooperation with Leonhard Grill's group, the researchers used the jointly developed surface polymerization and single-wire characterization (Science 2009, 323, 1193) to create molecular chains from alternating electron-rich and electron-poor units. The resulting alternating donor-acceptor polymers have excellent conductivity without loss of flexibility and in spite of the fact that the electrons are poorly distributed over the wire molecule.



The latter was unexpected and contradicts the commonly known model in which delocalization of the electrons over the molecule was the only guarantee for an efficient charge transport.

Stefan Hecht, a professor of organic chemistry and functional materials at the Humboldt-Universität zu Berlin, says, "Our study has contributed to the basic understanding of electronic transport by individual molecules and should help the design of new and better molecular wires," which, he hopes, will be an important impulse for the whole field of molecular and organic electronics.

This work was done within the framework of the EU project AtMol, "Atomic scale and single molecule logic gate technologies" in cooperation with researchers at Karl-Franzens-Univeristät Graz as well as at the French CNRS Institute CEMES in Toulouse and the Institute of Materials Research and Engineering (IMRE) in Singapore.

The results have been published in the journal Nature Communications:

Conductance of a single flexible molecular wire composed of alternating donor and acceptor units

C. Nacci, F. Ample, D. Bléger, S. Hecht, C. Joachim, and L. Grill Nature Communications 6 (2015) 7397 DOI: 10.1038/ncomms8397

Diffeomorphisms of Quantum Fields

Prof. Dirk Kreimer (HU, IRIS member) and Prof. Karen Yeats (U.Waterloo, visiting HU as a Senior Research Fellow of the Alexander von Humboldt Foundation) joined forces to understand the diffeomorphism invariance of quantum fields, and the interplay of such diffeomorphisms with renormalization schemes.



The vanishing of an on-shell connected Green function mandatesa relations between connected and one-particle-irreducible Green function

It has been observed since a long time that the formal invariance of the path integral usually employed to come to terms with the definition of amplitudes in quantum field theory is not fully established. The problem was studied combining the Hopf algebra structure of Feynman diagrams with an application of the theory of Bell polynomials. The results show that an invariance under diffeomorphisms of quantum fields can indeed be established when a renormalization scheme is employed which allows for a well-defined scattering matrix: amplitudes as solutions of quantum equations of motion must fulfill kinetic renormalization conditions: quantum corrections vanish for a prescribed set of momenta of scattering particles. For other renormalization schemes, the desired invariance of quantum fields is violated. This clarifies many misconceptions in the existing literature.

It does not only allow for a classification of renormalization schemes but allows for progress with foundational aspects of quantum field theory. A first paper has been recently finished. In the next couple of years Kreimer and Yeats plan to continue this work with an eye in particular to modern mathematical structures which appear here as undelying quantum field theory and the scattering theory of elementary particle theory.

Diffeomorphisms of quantum fields.

Dirk Kreimer, Karen Yeats arXiv:1610.01837 [math-ph] DOI: 10.1007/s11040-017-9246-0



Schematic illustration of the field-effect transistor based on blends of photochromic molecules bearing different alkyl substituents (shown in blue) blended with a small molecule organic semiconductor (shown in red). This blend results in high or low performance switch under illumination depending on the photochromic molecule.

Optically addressable transistors by mixing small molecule semiconductors and photoswitches

An international team of researchers led by Stefan Hecht (Member of IRIS Adlershof) and Paolo Samori from the Université de Strasbourg (France), in collaboration with scientists from Stanford University (USA) and the Université libre de Bruxelles (Belgium), demonstrated that high-performance optically switchable field-effect transistors can be developed by blending photochromic molecules with small organic semiconductor molecules. Such optically addressable molecular devices are considered as key elements in future logic circuits. Their study just appeared in the journal Nature Communications.

Organic optoelectronic materials attract particular attention for the development of low-cost multifunctional devices, such as phototransistors and optical memories. In these devices, light is used as a remote control to modulate electrical properties. In particular, conductivity can be tuned by incorporating photochromic molecules, which are able to undergo a reversible light-induced interconversion between two isomers possessing markedly different physical and chemical properties.

Diarylethenes (DAEs) are among the most interesting photochromic molecules to be embedded into thin-film transistors (TFTs) as a single semiconducting component. However, thin films made solely from DAEs suffer from rather poor charge transport properties. This problem can be solved by blending the DAE with organic semiconducting polymers in order to combine the light responsive nature of the DAE with the advantageous charge transport characteristics of the respective matrix component as reported in seminal work by the same team of scientists from Berlin and Strasbourg (see Nature Chemistry 4, 675 (2012)). This raised the question whether the approach of blending DAE with a polymer is general and also applicable to small semiconducting molecules, which are known to exhibit greater device performance when integrated in thin-film transistors.

Therefore, in this study, the researchers explored the effect of supramolecular organization mediated by the specific substitution pattern of the DAE on its photoswitching behavior when incorporated in both polymeric as well as small molecule matrices. Poly(3-hexylthiophene) (P3HT) was chosen as a model polymeric semiconductor, and a benzothienobenzothiophene (BTBT) derivative decorated with C_{12} alkyl chains was selected as the small molecule semiconducting matrix due to its exceptional electronic characteristics and solution processability.

The researchers were able to fabricate BTBT based optically switchable transistors with charge carrier mobilities as high as $0.21 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. Their results show that the molecular design made it possible to control the interactions between the blended components and thus the structure/morphology within the films, ultimately affecting the charge transport in the device as well as the current photomodulation and hence the overall switching performance.

They demonstrated that small molecule semiconductors can indeed outperform their polymeric counterparts in photoresponsive electrical performance when blended with DAE photochromic molecules in TFTs. Both DAE substitution pattern – which controls thin film morphology – and irradiation conditions – which need to maintain reversibility – turn out to be critical parameters for optimization.

Schematic illustration of the field-effect transistor based on blends of photochromic molecules bearing different alkyl substituents (shown in blue) blended with a small molecule organic semiconductor (shown in red). This blend results in high or low performance switch under illumination depending on the photochromic molecule.

These results prove that the originally developed blending approach is generally applicable to organic semiconducting molecules and can be tuned to fit the priority function of the device in question. These findings are attractive for the development of high-performing optically-gated electronic devices for potential applications in memories and logic circuits, and more generally in optoelectronics and optical sensing.

Optically switchable transistors by simple incorporation of photochromic systems into small molecule semiconducting matrices

M. El Gemayel, K. Börjesson, M. Herder, D. T. Duong, J. A. Hutchison, C. Ruzié, G. Schweicher, A. Salleo, Y. Geerts, S. Hecht, E. Orgiu, and P. Samorì *Nature Communications, 6 (2015) 6330* DOI: *10.1038/ncomms7330*

Reproducibility in density functional theory calculations of solids

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



types, to assess the quality of the equations of state for 71 elemental crystals. The overall conclusion is that predictions from recent codes and pseudopotentials agree very well, with

pairwise differences that are comparable to those between different high-precision experiments. Results of older methods, however, show stronger discrepancies. exciting, the program package [1,2] developed in the group of Claudia Draxl at the Humboldt-Universität zu Berlin (Physics Department and **IRIS Adlershof**) represents one of the all-electron full-potential implementations of DFT. It employs the linearized-augmented planewave basis, which is considered the gold standard within the condensed-matter community. Within this study, exciting has proven to be among the three most precise packages, with nearly negligible differences between them.

exciting has not only evolved into a benckmark code for DFT but has a strong focus on excitations that are treated within time-dependent DFT and many-body perturbation theory. In August 2016, HoW exciting! 2016 [3] took place at the Campus Adlershof, consisting of an international workshop on excitations in solids and a hands-on course employing exciting.

- [1] exciting-code.org
- [2] exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory
 A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti,
 S. Sagmeister, U. Werner, and C. Draxl
 J. Phys: Condes. Matter (Topical Review) 26 (2014) 363202
 DOI: 10.1088/0953-8984/26/36/363202
- [3] how-exciting-2016.physik.hu-berlin.de/

Reproducibility in density functional theory calculations of solids

K Lejaeghere, G Bihlmayer, T Bjoerkman, P Blaha, S Bluegel, V Blum, D Caliste, I. E. Castelli, S J Clark, A Dal Corso, S de Gironcoli, T Deutsch, J K Dewhurst, I Di Marco, C Draxl, M Dulak, O Eriksson, J A Flores-Livas, K F Garrity, L Genovese, P Giannozzi, M Giantomassi, S Goedecker, X Gonze, O Granaes, E K U Gross, A Gulans, F Gygi, D.R. Hamann, P J Hasnip, N A W Holzwarth, D Iusan, D B Jochym, F Jollet, D Jones, G. Kresse, K Koepernik, E Kuecuekbenli, Y O Kvashnin, I L M Locht, S Lubeck, M. Marsman, N Marzari, U Nitzsche, L Nordstrom, T Ozaki, L Paulatto, C J Pickard, W. Poelmans, M I J Probert, K Refson, M Richter, G.-M Rignanese, S Saha, M Scheffler, M Schlipf, K Schwarz, S Sharma, F Tavazza, P Thunstroem, A Tkatchenko, M Torrent, D. Vanderbilt, M J van Setten, V Van Speybroeck, J M Wills, J R Yates, G.-X Zhang, and S. Cottenier *Science 351 (2016) 1415* DOI: *10.1126/science.aad3000*

Enlightening and flexing memories

Researchers from Humboldt-Universität zu Berlin, led by Professor Stefan Hecht, who is a member of **IRIS Adlershof**, in collaboration with the Université de Strasbourg, CNRS (France) and the Univerza v Novi Gorici (Slovenia), have shown that a carefully chosen blend of a small photoswitchable molecule and a semiconducting polymer can be used to fabricate high-performance memory devices that can be written and erased by light. Such multilevel (8-bit) optical memories have also been implemented on flexible substrates, paving the way to applications in wearable electronics, E-papers, and smart devices. These results have been published in Nature Nanotechnology.

In the quest to improve the data storage capability of everyday electronic devices (randomaccess memories, hard disk drives, USB flash drives, etc.), alternative strategies to conventional silicon-based technologies need to be developed. The continuous miniaturization of electronic circuits, leading to the integration of a larger number of memory cells per unit area, has already shown its limitations due to the increased fabrication complexity. Another appealing approach consists in developing memory elements capable of storing not just one but multiple bits of information per device, commonly referred to as multilevel memories.

Now a European team of researchers from Berlin, Strasbourg, and Nova Gorica developed a light-responsive organic thin-film transistor by blending a custom-designed molecule serving as miniaturized optical switch with a high-performance semiconducting polymer. Upon illumination with ultraviolet and green light to "write" and "erase" information, respectively, the molecular switch undergoes a reversible interconversion between two distinct forms, one enabling and the other one preventing current to flow through the surrounding semiconducting polymer.



By integrating these components into transistor devices and using short laser pulses the researchers were able to construct multilevel memories with a data storage capacity of 8 bits. Importantly, their prototype devices combine high endurance over 70 write–erase cycles and data retention times exceeding 500 days.

Taking the work yet to another level, the team could transfer the device concept to flexible and lightweight polymer substrates, such as polyethylene terephthalate, to replace the commonly used rigid silicon. The resulting "soft" architecture preserves its electrical characteristics after 1000 bending cycles, thereby demonstrating its robustness and suitability for flexible electronics.

These findings are of great importance for the realization of high-performance smart and foldable electronic (nano)devices programmed by light with potential applications in flexible, multilevel high-density optical memories, logic circuits, and more generally in the next generation optoelectronics.

Flexible non-volatile optical memory thin-film transistor device with over 256 distinct levels based on an organic bicomponent blend

T. Leydecker, M. Herder, E. Pavlica, G. Bratina, S. Hecht, E. Orgiu, and P. Samorì Nature Nanotechnology 11 (2016) 769 DOI: 10.1038/nnano.2016.87

Tapping the sun

A team of researchers from IRIS Adlershof of the Humboldt-Universität zu Berlin and Technische Universiteit Eindhoven in the Netherlands have developed thin plastic films, which continuously move upon exposure to sunlight. These materials are able to convert the sunlight's energy directly into motion and have great promise for the development of sun-driven active coatings and surfaces, for example self-cleaning windows. These results have been published in Nature Communications. In order to harvest and utilize the sun's energy, alternative strategies to circumvent issues with energy storage and directly con-



Converting sunlight directly into motion by organizing light-responsive molecules, Figure: Dr. David Bléger

vert it into mechanical work have been developed over the years. A promising approach has been the design of light-driven molecular systems and machines; however, the collection of the individual molecules' response and subsequent amplification to macroscopic motion and mechanical work has proven difficult. Furthermore, previous systems required the use of intense high-energy UV light and therefore displayed poor performance in the context of solar energy conversion.

By carefully investigating the individual parameters of the system, the researchers found that the degree of oscillation depends on both the intensity and wavelength of the light and only occurs if both colors, i.e. blue and green triggering the opposite photoreactions, are present. As a result chaotic, macroscopic motion can be realized using "normal" sunlight, without the aid of specific optics or artificial light sources. The authors foresee immediate practical outdoor applications including self-cleaning coatings and surfaces, for example in windows. In general, these findings should be of great importance for the development of autonomous, sunlight-driven nano- and micromachinery.

A chaotic self-oscillating sunlight-driven polymer

K. Kumar, C. Knie, D. Bléger, M.A. Peletier, H. Friedrich, S. Hecht, D.J. Broer, M.G. Debije, and A.P.H.J. Schenning *Nature Communications 11975 (2016), published online* DOI: 10.1038/ncomms11975

Light controls repair of materials

A team of German researchers led by chemists of the Humboldt-Universität zu Berlin has developed a new type of plastic coating, which can heal damages selectively by illumination with light. A heat-induced repair of the material occurs where the damaged area has previously been illuminated with light of a specific color. The promising results of this work have now been published in Nature Communications.

To avoid the environmentally unfriendly as well as expensive replacement of damaged consumer products and constructions, researchers have recently been focusing their efforts on the development of smart materials able to self-repair scratches or cracks. Especially plastic coatings, which are repaired by heat, have yielded promising results in the past. Once subjected to heat, a chemical reaction induces melting and thus enables a homogeneous and complete mending. Upon cooling, the plastic re-establishes its original chemical structure as well as mechanical properties: It hardens and becomes robust again. However, the thermal stress during the healing procedure affects the overall material properties and eventually leads to degradation when applied repeatedly.

To bypass this problem, German researchers from the Humboldt-Universität zu Berlin, the Friedrich-Schiller-Universität Jena, the Federal Institute for Materials Research and Testing in Berlin as well as the Helmholtz-Zentrum Geesthacht in Teltow have now developed a smart plastic coating, in which light focusses the thermal healing process to the damaged locations only, without affecting the nondamaged parts.

"We aimed to protect intact parts of coatings from degradation.", says lead researcher Stefan Hecht and adds: "By employing light as stimulus, we now have a true remote control to switch the ability to self-repair 'on' or 'off' on demand." Shining light on damaged areas of the coating enables the self-repairing function. This process can be reversed by changing the color of the employed light yielding the original material – but in the healed state.



This seminal development is an important step to future applications in consumer products where light as a remote control facilitates external control over properties of smart materials. This could include the use as latent resists carried through various processing steps in nanofabrication or 3D printing.

Conditional repair by locally switching the thermal healing capability of dynamic covalent polymers with light

A. Fuhrmann, R. Göstl, R. Wendt, J. Kötteritzsch, M.D. Hager, U.S. Schubert, K. Brademann-Jock, A.F. Thünemann, U. Nöchel, M. Behl, and S. Hecht *Nature Communications 13623 (2016), published online* DOI: 10.1038/ncomms13623

Enhanced Photon Emission through optical Nano-fiber

An international team of researchers of the Humboldt-Universität zu Berlin (HU) led by a member of **IRIS Adlershof**, Prof. Oliver Benson and researchers of the Kyoto University in Japan demonstrated enhanced emission of individual particles of light - so-called photons - using a novel kind of structured nano-fibers. During the experiments not only an extraordinarily high number of photons was generated but also a precise adjustment of their wavelength was achieved. These tailored photons can be provided for applications in new quantum technologies directly through the fiber. The results have been published online in the current issue of the open access journal "Scientific Reports" of the Nature Publishing Group.

The structured nano-fiber represents a special kind of micro-resonator. Such resonators are used to study fundamental physical effects in the field of quantum optics. In analogy to a tuning fork, that stores sound waves, the micro-resonator stores light of a certain wavelength



Figure: a) Schematic of a structured nano-fiber. Note, that the number of grating-periods has been reduced here; b) scanning-ion-microscope-image of a nano-fiber (diameter 270 nm, depth of grooves 45 nm, distance of grooves 300 nm, and length of central defect 450 nm); c) electric field, numerically computed. The black line marks the boundary of the structured fiber; d) computed transmission spectrum.

over a relatively long time accompanied with an enhancement of the light intensity. Interaction between light and tiniest amounts of matter down to individual atoms can be investigated, controlled and utilized by this approach. The micro-resonators used here by the researchers have been patented already in 2010 in Japan, but it is only now, that it is possible to use them as the fabrication-process is very demanding. For the fabrication the researchers used a focused beam of Gallium ions to engrave tiny structures into the glass fiber, which is only a few hundred nanometers thick. This relates to a diameter that is more than a hundred times smaller than that of a human hair. Small semiconductor crystals of only a few nanometers in size served here as a photon source. These crystals have been placed in a controlled way onto the structured region of the nano-fiber. As a result, the light emission from the semiconductor crystals is enhanced and the photons are emitted directly into the glass fiber.

A micro-resonator can only store and enhance light of a specific wavelength. In order to couple this light with molecules or atoms, for example to realize a molecular or atomic switch, the resonator has to be aligned accurately. The researchers achieved this through a simple mechanism: by pulling they were able to deform the nano-fiber in a controlled way and by this to change the properties of the resonator deterministically. In a system with many different switching elements these elements can be aligned with respect to each other. A selective interplay of such elements would be the basis for an integrated optical quantum-chip, that is needed for quantum based calculations in a quantum-computer.

Currently, the researchers work on improvements of the micro-resonators and on ways to couple also optical emitters other than semiconductor crystals to the fibers. This would widen the range of potential applications, for example for save data transfer in telecommunication via quantum cryptography. Furthermore, a single molecule coupled to the fiber could be used as a nano-probe for sensing. Such a probe would represent the smallest sensor possible which may lead to so-far unrivalled precision in detecting tiniest amounts of matter.

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

4.2. Publications in important high impact journals

2015

Charge-transfer crystallites as molecular electrical dopants

H. Mendez, G. Heimel, S. Winkler, J. Frisch, A. Opitz, K. Sauer, B. Wegner, M. Oehzelt,
C. Roethel, S. Duhm, D. Toebbens, N. Koch, and I. Salzmann *Nat. Commun. 06 (2015), 8560*DOI: 10.1038/ncomms9560

Conductance of a single flexible molecular wire composed of alternating donor and acceptor units

C. Nacci, F. Ample, D. Bleger, S. Hecht, C. Joachim, and L. Grill Nat. Commun. 06 (2015), 7397 DOI: 10.1038/ncomms8397

Efficient light emission from inorganic and organic semiconductor hybrid structures by energy-level tuning

R. Schlesinger, F. Bianchi, S. Blumstengel, C. Christodoulou, R. Ovsyannikov, B. Kobin, K. Moudgil, S. Barlow, S. Hecht, S.R. Marder, F. Henneberger, and N. Koch *Nat. Commun. 06 (2015), 6754* DOI: *10.1038/ncomms7754*

Optically switchable transistors by simple incorporation of photochromic systems into smallmolecule semiconducting matrices

M. El Gemayel, K. Borjesson, M. Herder, D.T. Duong, J.A. Hutchison, C. Ruzie, G. Schweicher, A. Salleo, Y. Geerts, S. Hecht, E. Orgiu, and P. Samori *Nat. Commun. 06 (2015), 6330* DOI: *10.1038/ncomms7330*

Big Data of Materials Science: Critical Role of the Descriptor

L.M. Ghiringhelli, J. Vybiral, S.V. Levchenko, C. Draxl, and M. Scheffler Phys. Rev. Lett. 114 (2015), 105503 DOI: 10.1103/PhysRevLett.114.105503

Computing Equilibrium Shapes of Wurtzite Crystals: The Example of GaN

H. Li, L. Geelhaar, H. Riechert, and C. Draxl Phys. Rev. Lett. 115 (2015), 085503 DOI: *10.1103/PhysRevLett.115.085503*

Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme

S. Rigamonti, S. Botti, V. Veniard, C. Draxl, L. Reining, and F. Sottile *Phys. Rev. Lett.* 114 (2015), 146402 DOI: 10.1103/PhysRevLett.114.146402

Surface Structure of V2O3(0001) Revisited

F.E. Feiten, J. Seifert, J. Paier, H. Kuhlenbeck, H. Winter, J. Sauer, and H.-J. Freund *Phys. Rev. Lett.* 114 (2015), 216101 DOI: 10.1103/PhysRevLett.114.216101

Titration of Ce³⁺ lons in the CeO₂(111) Surface by Au Adatoms

Y. Pan, N. Nilius, H.-J. Freund, J. Paier, C. Penschke, and J. Sauer Phys. Rev. Lett. 115 (2015), 269901 DOI: 10.1103/PhysRevLett.115.269901

Ultrafast Nonlinear Response of Bulk Plasmons in Highly Doped ZnO Layers

T. Tyborski, S. Kalusniak, S. Sadofev, F. Henneberger, M. Woerner, and T. Elsaesser Phys. Rev. Lett. 115 (2015), 147401 DOI: 10.1103/PhysRevLett.115.147401

Coupled-mode approach to square-gradient Bragg-reflection resonances in corrugated dielectric waveguides

O. Dietz, G. Kewes, O. Neitzke, and O. Benson Phys. Rev. A 92 (2015), 043834 DOI: 10.1103/PhysRevA.92.043834

Practical implementation and evaluation of a quantum-key-distribution scheme based on the time-frequency uncertainty

M. Leifgen, R. Elschner, N. Perlot, C. Weinert, C. Schubert, and O. Benson *Phys. Rev. A 92 (2015), 042311* DOI: *10.1103/PhysRevA.92.042311*

Bound excitons and many-body effects in x-ray absorption spectra of azobenzene-functionalized self-assembled monolayers

C. Cocchi and C. Draxl Phys. Rev. B 92 (2015), 205105 DOI: 10.1103/PhysRevB.92.205105

Nanoscale transport of surface excitons at the interface between ZnO and a molecular monolayer

S. Friede, S. Kuehn, S. Sadofev, S. Blumstengel, F. Henneberger, and T. Elsaesser *Phys. Rev. B 91 (2015), 121415* DOI: *10.1103/PhysRevB.91.121415*

Nonresonant coherent control: Intersubband excitations manipulated by a nonresonant terahertz pulse

G. Folpini, D. Morrill, C. Somma, K. Reimann, M. Woerner, T. Elsaesser, and K. Biermann Phys. Rev. B 92 (2015), 085306 DOI: 10.1103/PhysRevB.92.085306

Optical spectra from molecules to crystals: Insight from many-body perturbation theory

C. Cocchi and C. Draxl Phys. Rev. B 92 (2015), 205126 DOI: 10.1103/PhysRevB.92.205126

Nonequilibrium structure of colloidal dumbbells under oscillatory shear

N. Heptner, F. Chu, Y. Lu, P. Lindner, M. Ballauff, and J. Dzubiella *Phys. Rev. E 92 (2015), 052311* DOI: *10.1103/PhysRevE.92.052311*

Acylhydrazones as Widely Tunable Photoswitches

D.J. van Dijken, P. Kovaricek, S.P. Ihrig, and S. Hecht JACS 137 (2015), 14982 DOI: 10.1021/jacs.5b09519

Adatoms underneath Single Porphyrin Molecules on Au(111)

J. Mielke, F. Hanke, M.V. Peters, S. Hecht, M. Persson, and L. Grill JACS 137 (2015), 1844 DOI: 10.1021/ja510528x

Improving the Fatigue Resistance of Diarylethene Switches

M. Herder, B.M. Schmidt, L. Grubert, M. Paetzel, J. Schwarz, and S. Hecht JACS 137 (2015), 2738 DOI: 10.1021/ja513027s

Synthesis, Structures, and Photophysical Properties of π -Expanded Oligothiophene 8-mers and Their Saturn-Like C₆₀ Complexes

H. Shimizu, J.D.C. Gonzalez, M. Hasegawa, T. Nishinaga, T. Haque, M. Takase, H. Otani, J.P. Rabe, and M. Iyoda JACS 137 (2015), 3877 DOI: 10.1021/jacs.5b00291

Tuning the Magnetic Properties of Carbon by Nitrogen Doping of Its Graphene Domains

Y. Ito, C. Christodoulou, M.V. Nardi, N. Koch, M. Klaeui, H. Sachdev, and K. Muellen JACS 137 (2015), 7678 DOI: 10.1021/ja512897m

A Heterobimetallic Superoxide Complex formed through O⁻² Activation between Chromium(II) and a Lithium Cation

F. Schax, S. Suhr, E. Bill, B. Braun, C. Herwig, and C. Limberg Angew. Chem. Int. Ed. 54 (2015), 1352 DOI: 10.1002/anie.201409294

A Structural and Functional Model for the 1-Aminocyclopropane-1-carboxylic Acid Oxidase

M. Sallmann, F. Oldenburg, B. Braun, M. Reglier, A.J. Simaan, and C. Limberg Angew. Chem. Int. Ed. 54 (2015), 12325 DOI: 10.1002/anie.201502529

Surface-Induced Selection During In Situ Photoswitching at the Solid/Liquid Interface

S. Bonacchi, M. El Garah, A. Ciesielski, M. Herder, S. Conti, M. Cecchini, S. Hecht, and P. Samori Angew. Chem. Int. Ed. 54 (2015), 4865

DOI: 10.1002/anie.201412215

Visible-Light-Activated Molecular Switches

D. Bleger and S. Hecht Angew. Chem. Int. Ed. 54 (2015), 11338 DOI: 10.1002/anie.201500628

Water Interaction with Iron Oxides

P. Dementyev, K.-H. Dostert, F. Ivars-Barcelo, C.P. O'Brien, F. Mirabella, S. Schauermann, X. Li, J. Paier, J. Sauer, and H.-J. Freund Angew. Chem. Int. Ed. 54 (2015), 13942 DOI: 10.1002/anie.201506439

Investigation of Line Width Narrowing and Spectral Jumps of Single Stable Defect Centers in ZnO at Cryogenic Temperature

O. Neitzke, A. Morfa, J. Wolters, A.W. Schell, G. Kewes, and O. Benson Nano Lett. 15 (2015), 3024 DOI: 10.1021/nl504941q

Nanophase Separation in Monomolecularly Thin Water-Ethanol Films Controlled by Graphene

N. Severin, J. Gienger, V. Scenev, P. Lange, I.M. Sokolov, and J.P. Rabe Nano Lett. 15 (2015), 1171 DOI: 10.1021/nl5042484

On-Demand Electrostatic Coupling of Individual Precharacterized Nano- and Microparticles in a Segmented Paul Trap

A. Kuhlicke, A. Rylke, and O. Benson Nano Lett. 15 (2015), 1993 DOI: 10.1021/nl504856w

Organic Non-Volatile Resistive Photo-Switches for Flexible Image Detector Arrays

S. Nau, C. Wolf, S. Sax, and E.J.W. List-Kratochvil Adv. Mater. 27 (2015), 1048 DOI: 10.1002/adma.201403295

Inkjet-Printed Resistive Switching Memory Based on Organic Dielectric Materials: From Single Elements to Array Technology

S. Nau, C. Wolf, K. Popovic, A. Bluemel, F. Santoni, A. Gagliardi, A. di Carlo, S. Sax, and E.J.W. List-Kratochvil *Adv. Electron. Mater. 1 (2015), 1400003* DOI: *10.1002/aelm.201400003*

The Effect of Gradual Fluorination on the Properties of $F_n ZnPc$ Thin Films and $F_n ZnPc/C_{60}$ Bilayer Photovoltaic Cells

M. Brendel, S. Krause, A. Steindamm, A.K. Topczak, S. Sundarraj, P. Erk, S. Hoehla, N. Fruehauf, N. Koch, and J. Pflaum Adv. Funct. Mater. 25 (2015), 1565 DOI: 10.1002/adfm.201404434

The Relationship between Structural and Electrical Characteristics in Perylenecarboxydiimide-Based Nanoarchitectures

C. Musumeci, I. Salzmann, S. Bonacchi, C. Roethel, S. Duhm, N. Koch, and P. Samori Adv. Funct. Mater. 25 (2015), 2501 DOI: 10.1002/adfm.201403773

The Impact of Disorder on the Energy Level Alignment at Molecular Donor-Acceptor Interfaces

K. Akaike, N. Koch, G. Heimel, and M. Oehzelt Adv. Mater. Interfaces 2 (2015), 1500232 DOI: 10.1002/admi.201500232

Double-soft limits of gluons and gravitons

T. Klose, T. McLoughlin, D. Nandan, J. Plefka, and G. Travaglini J. High Energy Phys. (2015), 135 DOI: 10.1007/jhep07(2015)135

From six to four and more: massless and massive maximal super Yang-Mills amplitudes in 6d and 4d and their hidden symmetries

J. Plefka, T. Schuster, and V. Verschinin J. High Energy Phys. (2015), 098 DOI: 10.1007/jhep01(2015)098

Local contributions to factorized soft graviton theorems at loop level

J. Broedel, M. de Leeuw, J. Plefka, and M. Rosso Phys. Lett. B 746 (2015), 293 DOI: 10.1016/j.physletb.2015.05.018

A beta 42-oligomer Interacting Peptide (AIP) neutralizes toxic amyloid-beta 42 species and protects synaptic structure and function

C. Barucker, H.J. Bittner, P.K.Y. Chang, S. Cameron, M.A. Hancock, F. Liebsch, S. Hossain, A. Harmeier, H. Shaw, F.M. Charron, M. Gensler, P. Dembny, W. Zhuang, D. Schmitz, J.P. Rabe, Y. Rao, R. Lurz, P.W. Hildebrand, R.A. McKinney, and G. Multhaup *Sci. Rep. 5 (2015), 15410* DOI: *10.1038/srep15410*

Highly Efficient Coupling of Nanolight Emitters to a Ultra-Wide Tunable Nanofibre Cavity

A.W. Schell, H. Takashima, S. Kamioka, Y. Oe, M. Fujiwara, O. Benson, and S. Takeuchi Sci. Rep. 5 (2015), 9619 DOI: 10.1038/srep09619

Micro-concave waveguide antenna for high photon extraction from nitrogen vacancy centers in nanodiamond

R. Rajasekharan, G. Kewes, A. Djalalian-Assl, K. Ganesan, S. Tomljenovic-Hanic, J.C. McCallum, A. Roberts, O. Benson, and S. Prawer *Sci. Rep. 5 (2015), 12013* DOI: *10.1038/srep12013*

2016

Reproducibility in density functional theory calculations of solids

K. Lejaeghere, G. Bihlmayer, T. Bjoerkman, P. Blaha, S. Bluegel, V. Blum, D. Caliste,
I.E. Castelli, S.J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J.K. Dewhurst, I. Di Marco,
C. Draxl, M. Dulak, O. Eriksson, J.A. Flores-Livas, K.F. Garrity, L. Genovese, P. Giannozzi,
M. Giantomassi, S. Goedecker, X. Gonze, O. Granaes, E.K.U. Gross, A. Gulans, F. Gygi,
D.R. Hamann, P.J. Hasnip, N.A.W. Holzwarth, D. Iusan, D.B. Jochym, F. Jollet, D. Jones,
G. Kresse, K. Koepernik, E. Kuecuekbenli, Y.O. Kvashnin, I.L.M. Locht, S. Lubeck,
M. Marsman, N. Marzari, U. Nitzsche, L. Nordstrom, T. Ozaki, L. Paulatto, C.J. Pickard,
W. Poelmans, M.I.J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler,
M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunstroem, A. Tkatchenko, M. Torrent,
D. Vanderbilt, M.J. van Setten, V. Van Speybroeck, J.M. Wills, J.R. Yates, G.-X. Zhang, and
S. Cottenier
Science 351 (2016), 1415
DOI: 10.1126/science.aad3000

A chaotic self-oscillating sunlight-driven polymer actuator

K. Kumar, C. Knie, D. Bleger, M.A. Peletier, H. Friedrich, S. Hecht, D.J. Broer, M.G. Debije, and A. Schenning

Nat. Commun. 7 (2016), 11975 DOI: 10.1038/ncomms11975

Conditional repair by locally switching the thermal healing capability of dynamic covalent polymers with light

A. Fuhrmann, R. Gostl, R. Wendt, J. Kotteritzsch, M.D. Hager, U.S. Schubert, K. Brademann-Jock, A.F. Thunemann, U. Nochel, M. Behl, and S. Hecht *Nat. Commun. 7 (2016), 13623* DOI: *10.1038/ncomms13623*

Chemistry in and out of nanoflasks

S. Hecht Nat. Nanotechnol. 11 (2016), 6 DOI: 10.1038/nnano.2015.274

Flexible non-volatile optical memory thin-film transistor device with over 256 distinct levels based on an organic bicomponent blend

T. Leydecker, M. Herder, E. Pavlica, G. Bratina, S. Hecht, E. Orgiu, and P. Samori Nat. Nanotechnol. 11 (2016), 769 DOI: 10.1038/nnano.2016.87

Comment on "Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme" Reply

S. Rigamonti, S. Botti, V. Veniard, C. Draxl, L. Reining, and F. Sottile *Phys. Rev. Lett.* 117 (2016), 159702 DOI: 10.1103/PhysRevLett.117.159702

Composite Operators in the Twistor Formulation of N=4 Supersymmetric Yang-Mills Theory

L. Koster, V. Mitev, M. Staudacher, and M. Wilhelm Phys. Rev. Lett. 117 (2016), 011601 DOI: 10.1103/PhysRevLett.117.011601

Mapping Atomic Orbitals with the Transmission Electron Microscope: Images of Defective Graphene Predicted from First-Principles Theory

L. Pardini, S. Loffler, G. Biddau, R. Hambach, U. Kaiser, C. Draxl, and P. Schattschneider *Phys. Rev. Lett.* 117 (2016), 036801 DOI: 10.1103/PhysRevLett.117.036801

Strong Amplification of Coherent Acoustic Phonons by Intraminiband Currents in a Semiconductor Superlattice

K. Shinokita, K. Reimann, M. Woerner, T. Elsaesser, R. Hey, and C. Flytzanis Phys. Rev. Lett. 116 (2016), 075504 DOI: 10.1103/PhysRevLett.116.075504

Two-Phonon Quantum Coherences in Indium Antimonide Studied by Nonlinear Two-Dimensional Terahertz Spectroscopy

C. Somma, G. Folpini, K. Reimann, M. Woerner, and T. Elsaesser Phys. Rev. Lett. 116 (2016), 7401 DOI: 10.1103/PhysRevLett.116.177401

Ab initio approach for gap plasmonics

U. Hohenester and C. Draxl Phys. Rev. B 94 (2016), 165418 DOI: 10.1103/PhysRevB.94.165418

Accurate all-electron G(0)W(0) quasiparticle energies employing the full-potential augmented plane-wave method

D. Nabok, A. Gulans, and C. Draxl Phys. Rev. B 94 (2016), 035118 DOI: 10.1103/PhysRevB.94.035118

Atomic signatures of local environment from core-level spectroscopy in beta-Ga2O3

C. Cocchi, H. Zschiesche, D. Nabok, A. Mogilatenko, M. Albrecht, Z. Galazka, H. Kirmse, C. Draxl, and C.T. Koch *Phys. Rev. B 94 (2016), 075147* DOI: *10.1103/PhysRevB.94.075147*

Observing single-atom diffusion at a molecule-metal interface

J. Mielke, J. Martinez-Blanco, M.V. Peters, S. Hecht, and L. Grill *Phys. Rev. B* 94 (2016), 035416 DOI: 10.1103/PhysRevB.94.035416

Probing the LDA-1/2 method as a starting point for G(0)W(0) calculations

R.R. Pela, U. Werner, D. Nabok, and C. Draxl Phys. Rev. B 94 (2016), 235141 DOI: 10.1103/PhysRevB.94.235141

Shift-current-induced strain waves in LiNbO3 mapped by femtosecond x-ray diffraction

M. Holtz, C. Hauf, A.A.H. Salvador, R. Costard, M. Woerner, and T. Elsaesser *Phys. Rev. B* 94 (2016), 104302 DOI: 10.1103/PhysRevB.94.104302

Tuning the work function of GaN with organic molecular acceptors

T. Schultz, R. Schlesinger, J. Niederhausen, F. Henneberger, S. Sadofev, S. Blumstengel, A. Vollmer, F. Bussolotti, J.P. Yang, S. Kera, K. Parvez, N. Ueno, K. Mullen, and N. Koch *Phys. Rev. B* 93 (2016), 125309 DOI: 10.1103/PhysRevB.93.125309

Reconstructing interaction potentials in thin films from real-space images

J. Gienger, N. Severin, J.P. Rabe, and I.M. Sokolov Phys. Rev. E 93 (2016), 043306 DOI: 10.1103/PhysRevE.93.043306

Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metal-Organic Frameworks

A. Kundu, G. Piccini, K. Sillar, and J. Sauer JACS 138 (2016), 14047 DOI: 10.1021/jacs.6b08646

Amides Do Not Always Work: Observation of Guest Binding in an Amide-Functionalized Porous Metal-Organic Framework

O. Benson, I. da Silva, S.P. Argent, R. Cabot, M. Savage, H.G.W. Godfrey, Y. Yang, S.F. Parker, P. Manuel, M.J. Lennox, T. Mitra, T.L. Easun, W. Lewis, A.J. Blake, E. Besley, S.H. Yang, and M. Schroder JACS 138 (2016), 14828 DOI: 10.1021/jacs.6b08059

Ultrafast Dynamics of Photoisomerization and Subsequent Unfolding of an Oligoazobenzene Foldamer

S. Steinwand, Z.L. Yu, S. Hecht, and J. Wachtveitl JACS 138 (2016), 12997 DOI: 10.1021/jacs.6b07720

Transparent Aluminium Oxide Coatings of Polymer Brushes

S. Micciulla, X. Duan, J. Strebe, O. Löhmann, R.N. Lamb, and R. von Klitzing Angew. Chem. 128 (2016), 5112 DOI: 10.1002/ange.201511669

AbInitio Calculation of Rate Constants for Molecule-Surface Reactions with Chemical Accuracy

G. Piccini, M. Alessio, and J. Sauer Angew. Chem. Int. Ed. 55 (2016), 5235 DOI: 10.1002/anie.201601534

Control of Imine Exchange Kinetics with Photoswitches to Modulate Self-Healing in Polysiloxane Networks by Light Illumination

M. Kathan, P. Kovaricek, C. Jurissek, A. Senf, A. Dallmann, A.F. Thunemann, and S. Hecht Angew. Chem. Int. Ed. 55 (2016), 13882 DOI: 10.1002/anie.201605311

Covalent Assembly and Characterization of Nonsymmetrical Single-Molecule Nodes

C. Nacci, A. Viertel, S. Hecht, and L. Grill Angew. Chem. Int. Ed. 55 (2016), 13724 DOI: 10.1002/anie.201605421

The Hydrated Excess Proton in the Zundel Cation $H_5O_2^+$: The Role of Ultrafast Solvent Fluctuations

F. Dahms, R. Costard, E. Pines, B.P. Fingerhut, E.T.J. Nibbering, and T. Elsaesser Angew. Chem. Int. Ed. 55 (2016), 10600 DOI: 10.1002/anie.201602523

Sensitized Two-NIR-Photon Z -> E Isomerization of a Visible-Light-Addressable Bistable Azobenzene Derivative

J. Moreno, M. Gerecke, L. Grubert, S.A. Kovalenko, and S. Hecht Angew. Chem. Int. Ed. 55 (2016), 1544 DOI: 10.1002/anie.201509111

Switching Diarylethenes Reliably in Both Directions with Visible Light

S. Fredrich, R. Goestl, M. Herder, L. Grubert, and S. Hecht Angew. Chem. Int. Ed. 55 (2016), 1208 DOI: 10.1002/anie.201509875

Transparent Aluminium Oxide Coatings of Polymer Brushes

S. Micciulla, X.F. Duan, J. Strebe, O. Lohmann, R.N. Lamb, and R. von Klitzing Angew. Chem. Int. Ed. 55 (2016), 5028 DOI: 10.1002/anie.201511669

Trapping Aluminum Hydroxide Clusters with Trisilanols during Speciation in Aluminum(III)-Water Systems: Reproducible, Large Scale Access to Molecular Aluminate Models

K.S. Lokare, N. Frank, B. Braun-Cula, I. Goikoetxea, J. Sauer, and C. Limberg Angew. Chem. Int. Ed. 55 (2016), 12325 DOI: 10.1002/anie.201604305

Light-Modulation of the Charge Injection in a Polymer Thin-Film Transistor by Functionalizing the Electrodes with Bistable Photochromic Self-Assembled Monolayers

T. Mosciatti, M.G. del Rosso, M. Herder, J. Frisch, N. Koch, S. Hecht, E. Orgiu, and P. Samori *Adv. Mater. 28 (2016), 6606* DOI: *10.1002/adma.201600651*

Dual-Characteristic Transistors Based on Semiconducting Polymer Blends

G.H. Lu, R. Di Pietro, L.S. Kolln, I. Nasrallah, L. Zhou, S. Mollinger, S. Himmelberger, N. Koch, A. Salleo, and D. Neher Adv. Electron. Mater. 2 (2016), 1600267 DOI: 10.1002/aelm.201600267

Effective Work Function Reduction of Practical Electrodes Using an Organometallic Dimer

K. Akaike, M.V. Nardi, M. Oehzelt, J. Frisch, A. Opitz, C. Christodoulou, G. Ligorio, P. Beyer, M. Timpel, I. Pis, F. Bondino, K. Moudgil, S. Barlow, S.R. Marder, and N. Koch *Adv. Funct. Mater.* 26 (2016), 2493 DOI: 10.1002/adfm.201504680

Coating of Vertically Aligned Carbon Nanotubes by a Novel Manganese Oxide Atomic Layer Deposition Process for Binder-Free Hybrid Capacitors

R.M. Silva, G. Clavel, Y.F. Fan, P. Amsalem, N. Koch, R.F. Silva, and N. Pinna Adv. Mater. Interfaces 3 (2016), 1600313 DOI: 10.1002/admi.201600313

Multidiffractive Broadband Plasmonic Absorber

I. Khan, H. Keshmiri, F. Kolb, T. Dimopoulos, E.J.W. List-Kratochvil, and J. Dostalek *Adv. Opt. Mater. 4 (2016), 435* DOI: 10.1002/adom.201500508

Switching to Bright

H. Tian and S. Hecht Adv. Opt. Mater. 4 (2016), 1320 DOI: 10.1002/adom.201600638

All tree-level MHV form factors in N=4 SYM from twistor space

L. Koster, V. Mitev, M. Staudacher, and M. Wilhelm J. High Energy Phys. (2016), 162 DOI: 10.1007/jhep06(2016)162

Einstein-Yang-Mills from pure Yang-Mills amplitudes

D. Nandan, J. Plefka, O. Schlotterer, and C.K. Wen J. High Energy Phys. (2016), 070, 1 DOI: 10.1007/jhep10(2016)070

Cooperative Switching in Nanofibers of Azobenzene Oligomers

C. Weber, T. Liebig, M. Gensler, A. Zykov, L. Pithan, J.P. Rabe, S. Hecht, D. Bleger, and S. Kowarik *Sci. Rep. 6 (2016), 25605* DOI: *10.1038/srep25605*

Organic heterojunctions: Contact-induced molecular reorientation, interface states, and charge redistribution

A. Opitz, A. Wilke, P. Amsalem, M. Oehzelt, R.-P. Blum, J.P. Rabe, T. Mizokuro, U. Hoermann, R. Hansson, E. Moons, and N. Koch *Sci. Rep. 6 (2016), 21291* DOI: *10.1038/srep21291*

A realistic fabrication and design concept for quantum gates based on single emitters integrated in plasmonic-dielectric waveguide structures

G. Kewes, M. Schoengen, O. Neitzke, P. Lombardi, R.S. Schonfeld, G. Mazzamuto, A.W. Schell, J. Probst, J. Wolters, B. Lochel, C. Toninelli, and O. Benson *Sci. Rep. 6 (2016), 28877* DOI: *10.1038/srep28877*

Wiring up pre-characterized single-photon emitters by laser lithography

Q. Shi, B. Sontheimer, N. Nikolay, A.W. Schell, J. Fischer, A. Naber, O. Benson, and M. Wegener *Sci. Rep. 6 (2016), 31135* DOI: *10.1038/srep31135*

4.3. Scientific Conferences and Seminars

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

Symposium "IRIS 2015"

July 10, 2015

Five years after its opening, the Integrative Research Institute for the Sciences **IRIS Adlershof**, hosted the one-day symposium IRIS 2015. The purpose of the symposium was to explore ideas how to further develop IRIS.



For instance, a physicist, a mathematician and computer scientist discussed opportunities Mathematical Physics of Complex Systems may offer for **IRIS Adlershof**. Other topics covered in the symposium included further developments in the research field of Hybrid Systems, its relations to Analytical Sciences and Biological Physics, as well as interactions between Cultural Studies and Natural Sciences.

Symposium "Polymer research in Berlin-Brandenburg"

October 30, 2015

The Berlin-Brandenburg Association for Polymers (BVP) held its biannual Regional Symposium at Humboldt-Universität's Campus Adlershof, featuring presentations from Universities, Institutes of the Max-Planck-society, the Helmholtz-Association, and the industry. The Symposium was organized by IRIS Adlershof.



Symposium on Chemistry & Physics of Macromolecules

November 20, 2015

Macromolecules, the dominating source in nature, play also a crucial role in a wide variety



of industries. Natural Sciences are the key to analyse and understand their complex properties, which are unachievable by other materials, and design more and more specialised molecules and systems for further applications. The symposium was intended to feature a few but fine selected presentations on cutting-edge research on the physics and chemistry of functional (macro-) molecules.

IR FAR

"Science meets business" – Advanced Materials

December 8, 2015

On 8 December 2015 Humboldt-Universität zu Berlin, Humboldt-Innovation GmbH and Berlin Partner presented the 4th knowledge and technology

transfer event of the series Wissenschaft trifft Wirtschaft (WtW, "Science meets business"). The 2015 event focused on Advanced Materials.

Main areas of research:

Physics:

- (Elementary) particle physics
- Solid state physics
- Macromolecules/complex systems
- Optics/photonics

Chemistry:

- Chemical biology
- Functionally structured materials and catalysis

The new event format aims at bringing together research and application. Companies were invited to present their research questions in the field of Advanced Materials as a short pitch

to an audience of scientists and other (local) businesses. At the event, researchers had the chance to learn about current and future challenges companies face working with new materials. At the same time, HU scientists from the Integrative Research Institute for the Sciences **IRIS Adlershof** and the Physics and Chemistry Departments were going to showcase their successful application-oriented research cooperations with third parties. Scientists and companies had ample opportunity to network and to discuss their research subjects in more detail in the course of the day.

"Hybrid-Photovoltaics 2015 Symposium"

December 10-11, 2015



The "Hybrid-Photovoltaics 2015 Symposium" was the concluding event of the Helmholtz Energy Alliance "Hybrid photovoltaics".

The topics of Symposium included:

- 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
- Perovskite solar cells

Kosmos Summer University on "Integrability for the Holographic Universe"

August 15 – September 2, 2016

K C S M O S HUMBOLDT-UNIVERSITÄT ZU BERLIN

Integrability has played a major role in the historical development of theoretical physics. Newton was able to exactly derive the Kepler laws from his novel theory of mechanics and gravity. Quantum mechanics established itself as a mathematically and physically correct theory through the exact solution of the idealized hydrogen atom. In both cases, the hidden



conservation of the Laplace-Runge-Lenz vector underlies these successes. Thus, the integrability of the central force problem is related to breakthroughs in both classical and quantum mechanics. It is widely felt that a similarly idealized model is needed to uncover the mysteries of gauge and string theory in general, and the intricate mechanism of the holographic principle in particular. This was the core topic of the "Integrability in Gauge and String Theory" (IGST) conference series, whose 2016 edition took place in Berlin.

The focus of the Kosmos Summer University 2016 was on integrability in holographic systems such as the AdS/CFT correspondence in various dimensions. Recent years have seen spectacular progress on both the gauge and string theory sides of certain holographically dual models, allowing for exact computations of operator spectra, scattering problems, correlation functions, and Wilson loops. The latest developments will be reviewed at this conference. Emphasis is on the solution of specific problems, but the mathematical structures underlying integrability are explored as well. Closely related topical fields such as lattice approaches, QCD string modeling, entanglement entropy studies and general CFT approaches will also be represented.

The KOSMOS Summer University 2016 was divided into three parts:

- Mathematica Summer School on Theoretical Physics, 15 19 August 2016,
- IGST 2016, 22 26 August 2016
- Focus Program, 29 August 2 September 2016

Prof. Nima Arkani-Hamed from the Institute of Advanced Studies at Princeton University held a public Kosmos lecture on "Physics and Mathematics for the End of Spacetime" in the Audimax of the main building of Humboldt-Universität zu Berlin.

Advanced Materials Competition (AdMaCom)

August 28 - October 10, 2016

As their first big internationally visible activity, the Innovation Network for Advanced Materials (INAM) has organized the Advanced Materials Competition (AdMaCom), which was a six-week workshop for developing innovative product concepts with international start-ups. Established companies like OSRAM, LG, Ledvance, and Henkel



have been providing the technological infrastructure, know-how and/or sponsoring. The 15 participating international and Berlin start-ups have taken advantage of this to improve their existing products and create new concepts.

The participants were able to draw upon the expertise of mentors from renowned international research facilities and industrial companies like LG Technology Center Europe, BASF Ventures, the London School of Economics, the Imperial College London as well as from Berlin like OSRAM, Direct Photonics Industries, Specs Nano Surface Analytics, Fab Lab Berlin, Humboldt-Universität's **IRIS Adlershof**, Humboldt Innovation, ESMT, WISTA and Berlin Partner. Berlin should be visualized as an international high tech location not only for start-ups but also for innovative departments from large companies. AdMaCom has been held under the patronage of the governing Mayor of Berlin.

Selected IRIS Colloquia

2015

- March 09: Dr. Tim Schröder, Quantum Photonics Laboratory Massachusetts Institute of Technology
 "Diamond Photonics: Quantum Devices, Nanostructures, and Sensing Photonic
- Quantum Networks based on Spin Qubits in Diamond"April 01: Prof. Dr. Steven L. Bernasek, Department of Chemistry, University of
- April 01: Prof. Dr. Steven L. Bernasek, Department of Chemistry, University of Princeton

"Structure and Dynamics in the Surface Chemical Bond"

 August 14: Prof. Dr. Bruce Parkinson, University of Wyoming, Laramie, WY USA "The Combinatorial Search for Semiconducting Oxides that Photoelectrolyze Water"

- May 24: Prof. em. Steve Granick, IBS Center for Soft and Living Matter, South Korea, Prof. Emeritus, University of Illinois, USA "Some Surprises and Open Questions in Soft Matter"
- November 02: Prof. Dr. Stefan Maier, Imperial College London "Plasmonic and dielectric nanoantennas: a versatile platform for interdisciplinary nanophotonics"
- November 17: Prof. Barry P. Rand, Princeton University "Controlling thin film organic and metal halide perovskite crystallinity and morphology to gain a better understanding of devices"

2016
5. Promotion of Young Scientists

As in the previous years IRIS members were involved in teaching classes of their corresponding departmental institutes. With special lectures that go into detail about the IRIS research areas, it is thus possible to interest student in the scientific work of **IRIS Adlershof** and to integrate master and doctoral students in **IRIS Adlershof** research projects.

IRIS Adlershof has directly supported young scientists during the reporting period. Several early stage researchers were given start-up and interim funds that were financed by **IRIS Adlershof**.

In 2015 and 2016 **IRIS Adlershof** organized a series of seminars on scientific writing targeting to early career 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.

On the initiative of the CRC 951 two coaching workshops for female IRIS- and SALSA young scientists were organized. The courses focused on "Team work & leadership competencies in academia and beyond" and "Networking in the academic context".

IRIS Adlershof's young scientists had impressive and successful results in the report period:

Dr. Claire Glanois has been awarded an Alexander von Humboldt Research Fellowship for Postdocs. Starting April 2017 she will join the group of Prof. Kreimer. She received her PhD in mathematics in January 2016 from the Université Pierre et Marie Curie (Paris) and is currently a postdoc at the MPI Mathematics in Bonn. The number theorist concentrates on periods as they appear in computations in quantum field theory, a central topic in Prof. Kreimer's group.

Dr. Lorenzo Bianchi, former member of the Emmy-Noether Junior Research group of Dr. Valentina Forini in the working group of Prof. Jan Plefka, has been awarded the Carl-Ramsauer-Prize 2016 of the Physikalische Gesellschaft zu Berlin for his outstanding PhD thesis on perturbation theory for string sigma models. This is an active research field to which Bianchi contributed by developing new powerful techniques, allowing for substantial simplifications in perturbative computations. Using these innovative methods several new results in the strong coupling regime of the AdS/CFT correspondence have been obtained.

Dr. Sven Ramelow started in fall 2016 to establish an Emmy Noether Junior Research Group on the topic of "Mid-Infrared Quantum Imaging and Spectroscopy" at Humboldt-Universität's Physics Department. He closely cooperates with the Nano-Optics-Group led by Prof. Oliver Benson. Parts of the basic equipment required by Dr Ramelow's Group were financed by IRIS.

The dissertation of Dr. Raphael Schlesinger was selected to be published in Springer Theses, a dedicated book series to recognize outstanding doctoral research. Raphael's work, conceived and performed within the CRC 951 at the physics department and IRIS Adlershof of Humboldt-Universität zu Berlin, was supervised by Prof. Norbert Koch, who is the deputy chairman of IRIS Adlershof.

6. Honors and Awards

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

- Prof. Dr. Thomas Elsässer: Lifetime Achievement Award 2015 of the Time Resolved Vibrational Spectroscopy Meeting (TRVS)
- Dr. Lorenzo Bianchi (Forini group): Italian Physical Society 2015 Prize "Giuliano Preparata" for a young graduate student

Carl-Ramsauer-Prize 2016 of the Physikalische Gesellschaft zu Berlin for his outstanding PhD thesis

- Dr. Valentina Forini: Journal of Physics A Highlight Paper of 2015 for: One-loop spectroscopy of semi classically quantized strings: bosonic sector Laboratory (FUNSOM), Soochow University, China
- Prof. Johann-Christoph Freytag, Ph.D.: Election as a member of the executive committee of the Gesellschaft für Informatik (GI) e.V. (2016)











Imprint

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