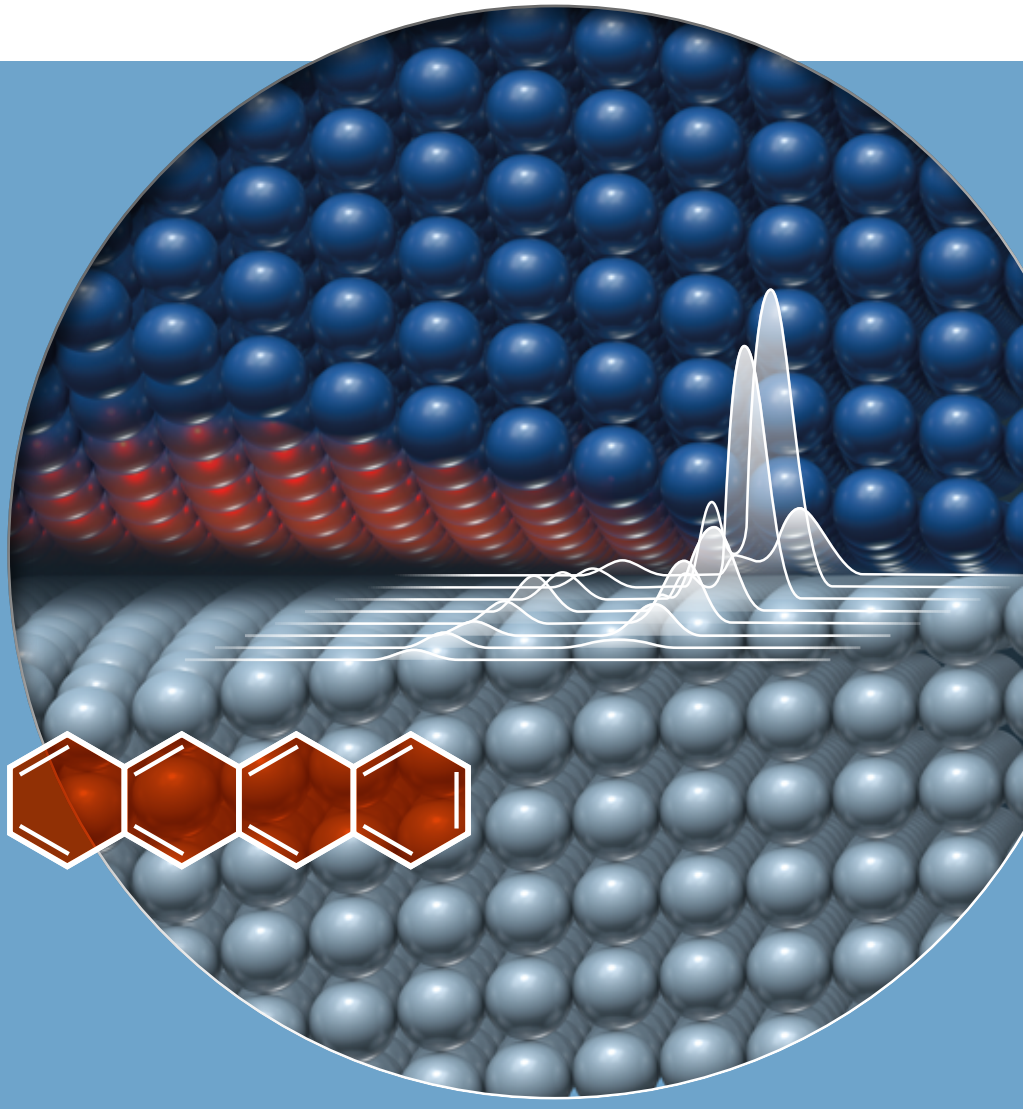
SFB 1083
Structure and Dynamics
of Internal Interfaces

Activity Report

2013–2019



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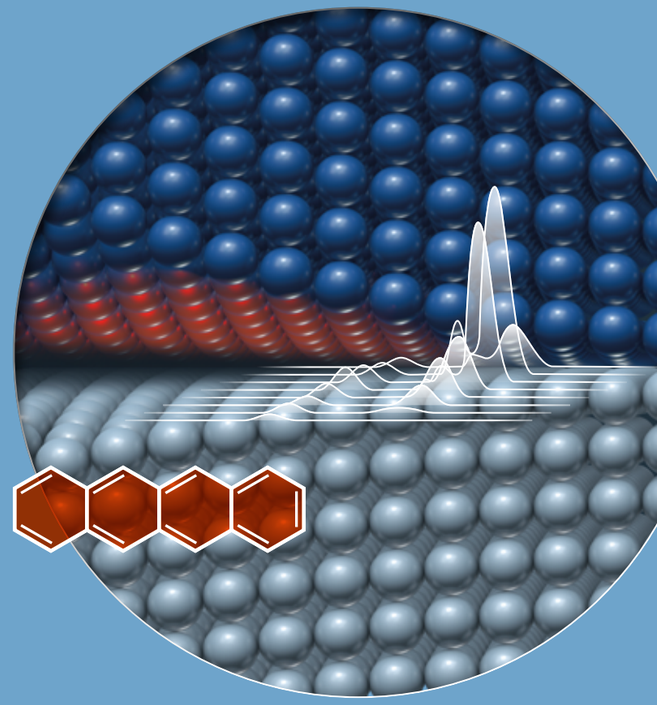
Content

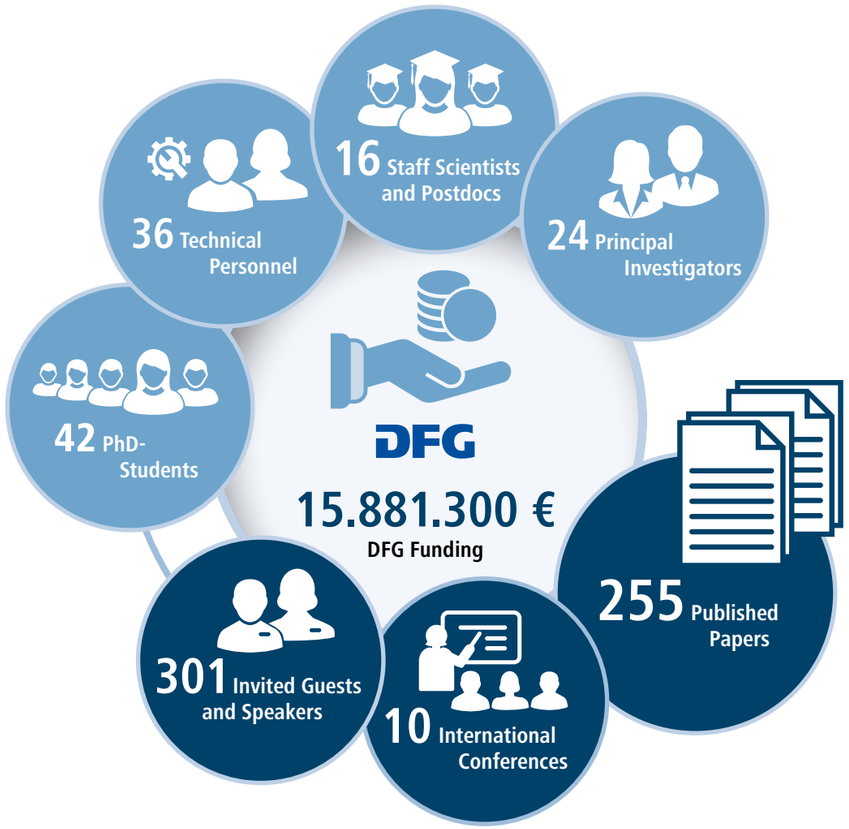
INTRODUCTION



The Interface is the Device.

This phrase coined by Herbert Kroemer in his Nobel lecture in the year 2000 states, that in many modern electronic devices the action takes place at the interface between two materials. It applies for transistors in microchips of our computers as well as for many other devices like solar cells, sensors, new displays and for many novel devices that might come up in the future. Despite their enormous importance, our microscopic understanding of internal interfaces is lagging behind that of volume or surface properties. The main reason for this knowledge gap is the experimental difficulty to detect and isolate the weak interface signature from the signals of the dominant bulk.

The objective of the collaborative research center SFB 1083 is to close this knowledge gap by collaboration between researchers from different fields. SFB 1083 has been established by the Deutsche Forschungsgemeinschaft at the Philipps-Universität Marburg in the year 2013. It consisted of 15 working groups in the fields of chemical synthesis, semiconductor physics, surface science, structural analysis and laser spectroscopy at the Departments of Physics and Chemistry of Philipps-Universität Marburg and a project at the Donostia International Physics Center in San Sebastián, Spain. After a successful first funding period from October 2013 to June 2017, the center now includes groups from Gießen, Jülich and Münster in its second funding period (July 2017 to June 2021). Presently SFB 1083 consists of 18 scientific projects and with about 80 scientists. The annual budget received from the DFG is about 2.5 Mio Euro complemented by core funding of the supporting institutions of about 1.5 Mio Euro per year.



"Primarily, our research is not directed towards specific functional materials, as those generally consist of many, frequently not well-defined interfaces. Instead, we focus on model systems with specially prepared internal interfaces. We structurally characterize these interfaces on the atomic level and investigate their optical and electronic properties systematically. In this way, we want to achieve a detailed microscopic understanding of chemical bonding, electronic coupling and energy transfer for different classes of heterointerfaces. We then can make use of this knowledge and tailor interfaces for specific applications and construct devices with novel properties and functions."

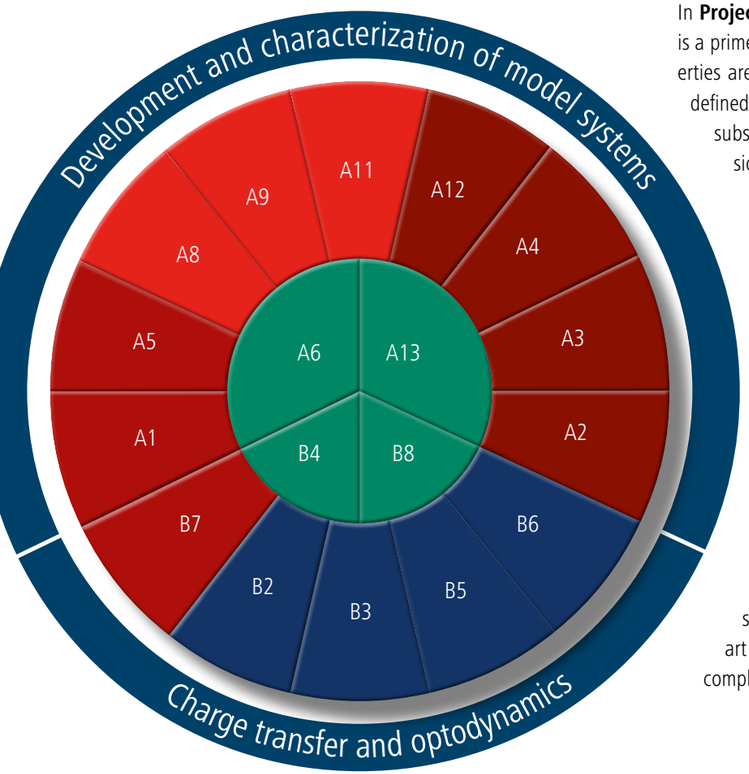
Ulrich Höfer, initiator and present spokesman of SFB 1083

Scope of SFB 1083

Internal interfaces in the sense of this collaborative research centre are interfaces between two solids. They are locations where two different electron systems couple. The research of SFB 1083 is focused on the detailed microscopic understanding of this coupling and how it can be influenced and tailored to specific needs. Since not only existing electronic semiconductor devices, but also most future applications of novel solid state materials, such as molecular or two-dimensional solids, rely on interfacial properties, research on internal interfaces lies at the heart of modern materials science. The material systems under investigation in SFB 1083 are inorganic semiconductors, organic thin films and metals. The particular choice of material combinations and interfaces between them is generally not driven by specific applications. Their choice is rather determined by their suitability as model systems to address and isolate fundamental processes of chemical and physical interactions at and across the interface.

The research program proceeds along three main lines. Two of these are directly reflected in the topic areas of the centre

A: Development and characterization of model systems,
B: Charge transfer and optodynamics.

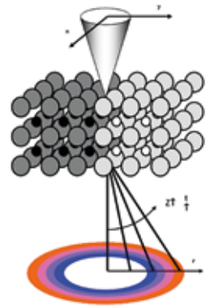


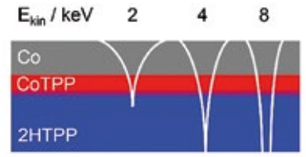
The structural analysis of internal interfaces, as well as the study of dynamical processes occurring at these interfaces, crucially depends on the availability of sensitive, interface-specific experimental methods. Thus, the development of such methods is the third major task of the SFB 1083. It is an important aspect of several projects in both topic areas.

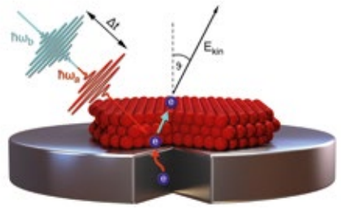
In **Project Area A**, material design and thin film growth is a prime task. New organic molecules with special properties are designed and synthesized. Using epitaxy, well defined interfaces are grown, often on single crystals as substrates. For characterization, scanning transmission electron microscopy plays an important role, particularly for inorganic materials when atomic resolution can be achieved. Photoelectron spectroscopy, a very powerful method for surface studies, is also applied. Both, for low and high electron energies the escape depth is large enough to probe the interface between two solids.

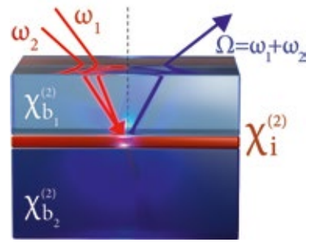
In **Project Area B**, laser spectroscopy plays a key role. With light interfaces can be accessed in a non-invasive way. If non-linear techniques are used, the weak interface signal can be isolated from the often dominant bulk. A particular strength of SFB 1083 is time-resolved spectroscopy of interfaces with state-of-the-art pump-probe methods. Theoretical experiments complete the expertise in both project areas.

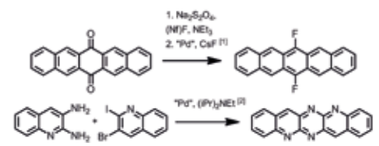
● semiconductor physics ● chemical synthesis ● surface science ● laser-spectroscopy ● theory/modelling











Characterization: Structure and Composition

- (Scanning) Transmission electron microscopy ((S)TEM)
- X-ray diffraction (XRD)
- Infrared spectroscopy (FTIR)

Photo Electron Spectroscopy

- Two-photon photoemission (2PPE)
- Hard X-ray photoelectron spectroscopy (HAXPES)

Time-Resolved Spectroscopy

- Optical pump-probe spectroscopy
- Time-resolved THz spectroscopy

Optical Spectroscopy

- Coherent phonon spectroscopy
- Second-harmonic and sum-frequency generation (SHG/SFG)

Material Design and Thin Film Growth

- Organic synthesis
- Metal organic vapor phase epitaxy (MOVPE)
- Organic molecular beam deposition (OMBD)

Theory

- Electronic structure calculations
- Electron, exciton, vibrational dynamics

As this Activity Report documents, SFB 1083 has significantly advanced the level of understanding of the structural properties of different classes of internal interfaces in the past six years. The following examples briefly exemplify this progress. A more detailed account is given in the Highlights section.

1. Structure of GaP/Si(001)

An interesting and important structural issue of all solid/solid interfaces is the degree of intermixing of both materials. For covalently bound semiconductor heterointerfaces, one generally expects some kind of interdiffusion of the two components, except when the two materials have the same lattice constant. Then common models predict an atomically abrupt interface. For GaP/Si(001), a prototype of such a lattice-matched system, the analysis of atomically resolved scanning transmission electron microscopy (STEM) data, however, reveals a characteristic, intrinsic pyramidal structure extending over several lattice planes. The result can be understood analogously to the reconstruction of surfaces where the interplay of different forces sometimes leads to extensive rearrangement of atoms from their positions in the volume. For GaP/Si, the pyramidal structure minimizes the sum of the local strain and the electrostatic forces of the polar/nonpolar interface. The results have important general consequences. Obviously, there are intrinsic limits as to the abruptness of interfaces between common semiconductors, irrespective of the conditions applied during their growth.

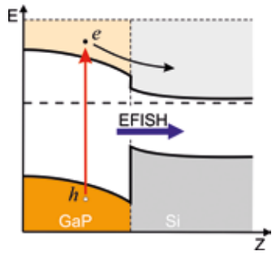
2. Organic/metal interface states

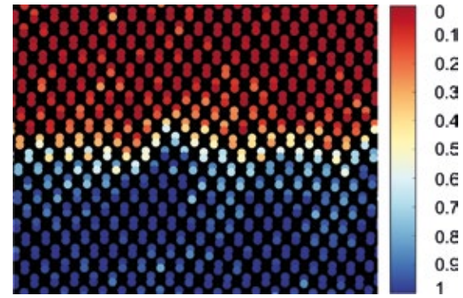
Interface-specific electronic states between a single-crystal metal and a well-ordered organic thin film were first reported by the Tautz group in Jülich and the Höfer group in Marburg for PTCDA/Ag(111) already several years before the SFB 1083 has been established. Related interface states have meanwhile been identified for a variety of weakly interacting organic/metal interfaces. The successful establishment of SFB 1083 and the subsequent close experiment theory collaboration has improved the general understanding and theoretical description of these new types of electronic states substantially. They resemble in many respects the Shockley surface states of clean metals although the existence of a Shockley state is not a prerequisite for the formation of interface states. The maximum probability density of the wave-function is located between the molecules of the first layer and the metal. On the one hand, a large overlap with the metal substrate leads to high lateral mobility of the electrons in the states. On the other hand, the probability density in the vicinity of the molecules of the first layer is laterally strongly corrugated and reflects the orbital structure of the molecules. Recently, time-resolved 2PPE experiments could clearly show that interface states can very efficiently mediate the electron transfer between a metal and an organic semiconductor when they are located between the Fermi-level of the metal and the molecular LUMO-orbital.

3. Organic/Si(001) interface

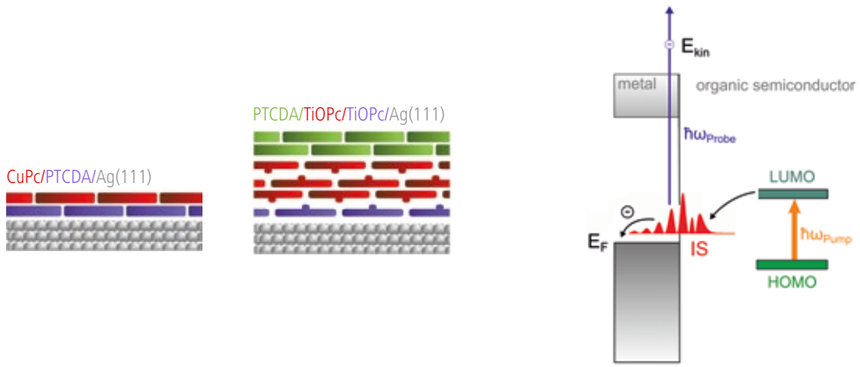
The combination of organic functionalities and inorganic semiconductors opens many interesting new opportunities in optoelectronics, for solar energy conversion, or as biosensors. A very challenging problem, however, is the controlled fixation of the organic molecules with specific functional groups at the semiconductor. Some substrates, like TiO_2, are rather inert and make the reliable covalent attachment difficult. Others, like silicon, have highly reactive dangling bonds at their surfaces which present a major hindrance for chemoselective attachment. Here, a major breakthrough could be achieved by adopting a strategy from chemical biology and employing cyclooctyne derivatives. It could be shown that model molecules, with ether and ester functionalization, adsorb selectively on Si(001) by a [2+2] cycloaddition via the strained cyclooctyne triple bond while leaving the functional side groups unreacted. The origin of the achieved selectivity is the direct adsorption pathway of cyclooctyne, as opposed to the vast majority of other organic functionalities. Their reaction with Si(001) generally proceeds via metastable intermediates, which makes them effectively unreactive in competition with the much faster direct pathway. With functionalized cyclooctynes a defined interface between silicon and a large variety or organic layers has thus been developed. This opens the road to the controlled organic functionalization of silicon by chemoselective layer-by-layer growth utilising click reactions.

Structure of GaP/Si(001)

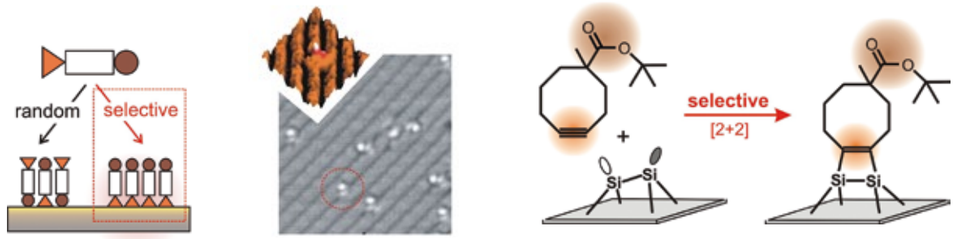




Organic/metal interface states



Organic/Si(001) interface



4. Interface excitions

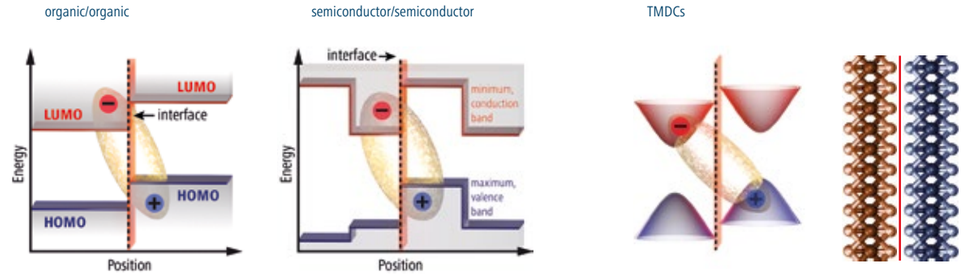
Charge-transfer (CT) excitons, where electron and hole reside in different materials and interact across the interface, constitute one of the fundamental quasi-particles at interfaces. This type of interface excitons are known to exist at semiconductor interfaces where they are called type-II excitons. Using optical pump, THz probe experiments, researchers of SFB 1083 investigate the dynamics of such interface excitons in the time domain. Charge transfer excitons also exist at interfaces of organic donor/acceptor systems. There, they are frequently postulated to play an important role for the charge separation in organic solar cells. The non-regularity of most organic/organic interfaces, such as those between polymer blends, however, has hampered not only the microscopic characterization of such CT excitons, but also a clear spectroscopic confirmation of their existence. Researchers of SFB 1083 succeed to establish several model systems or organic donor/acceptor systems where they have full control of the morphology of these interfaces. This has enabled the clear spectroscopic identification of interface transitions in two systems and correlate the properties of CT-excitons with the interface structure. As a new aspect, SFB 1083 extended these studies to interfaces of transition metal dichalcogenides and other novel two-dimensional materials. Van der Waals heterostructures based on these materials offer completely new perspectives for materials design. Many properties of these future materials will be interface-dominated.

5. Type-II semiconductor laser

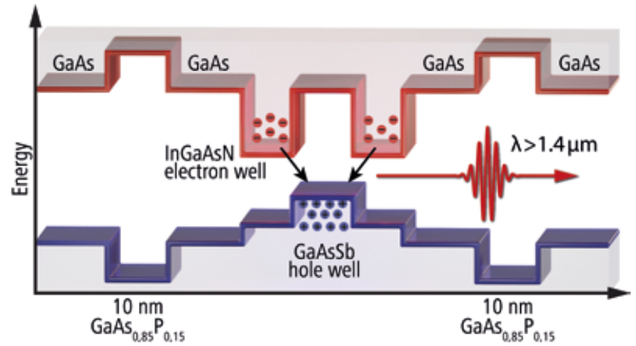
Conventional semiconductor lasers operating at long wavelengths are difficult to realize because Auger-losses dominate low energy transitions in narrow-gap materials. It has been suggested that this problem may be circumvented with so-called W-structures. These consist of quantum wells with normal band gaps and make use of optical transitions across a type-II interface for laser operation. Soon after establishment of SFB 1083 it could be shown that this is indeed a very promising concept to facilitate laser operation at wavelengths of 2 µm and beyond. With carefully designed interface roughness, type-II transitions across interfaces are surprisingly strong. In the meantime Watt level output powers have already been demonstrated at 1.2 µm.

SFB spokesman Prof. Dr. Ulrich Höfer (right) explains an optical setup to investigate internal interfaces to vicepresident for reseach Prof. Dr. Ulrich Koert, and to SFB vice-spokeswomen Prof. Dr. Kerstin Volz in Mai 2013, shortly after DFG granted funding of the center.

Interface excitions



Type-II semiconductor laser

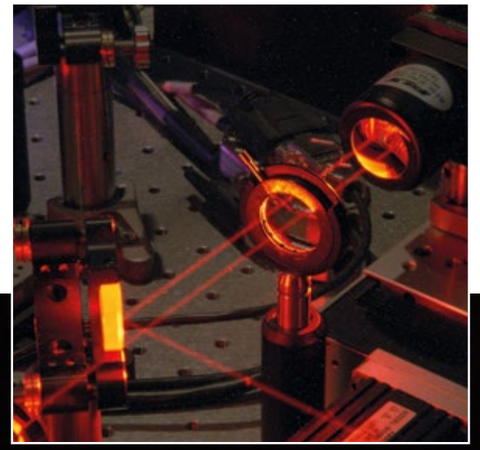


Main general tasks and goals of SFB 1083:

- characterize the structure of different classes of internal interfaces with atomic precision
- understand the characteristics of chemical bond formation at heterointerfaces
- experimentally determine electronic properties, such as level alignment or interface states
- detect interface-specific vibrational properties
- theoretically predict structural, electronic and optodynamical properties
- understand the mechanisms of charge and energy transfer across interfaces
- tailor interfaces to specific needs by applying this knowledge
- create prototypes of new materials or devices.

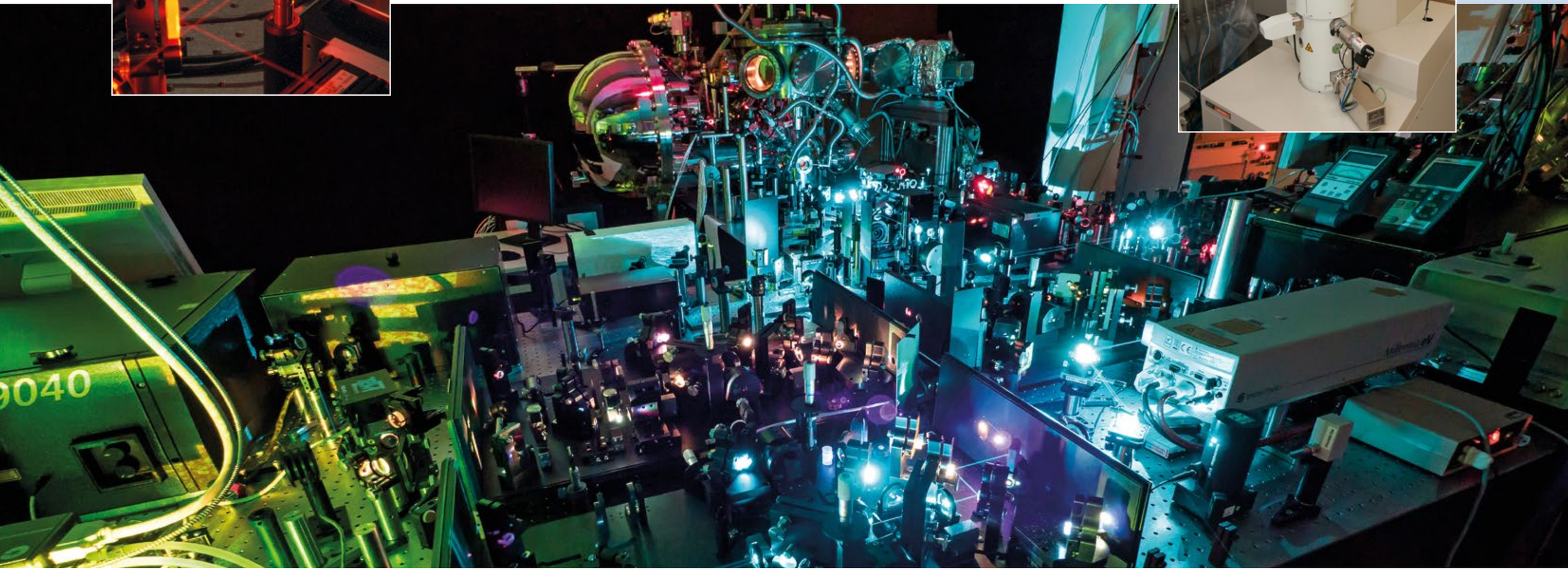
Research Infrastructure

The groups of SFB 1083 have access to state-of-the-art instrumentation to accomplish their research. This includes apparatus to grow well-defined layers and internal interfaces as well as instruments to characterize these model systems and to investigate their optoelectronic properties.

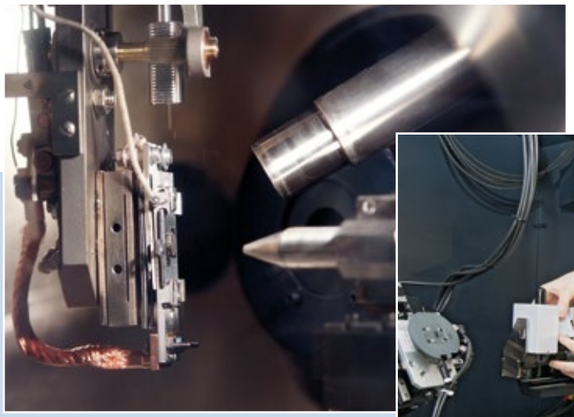


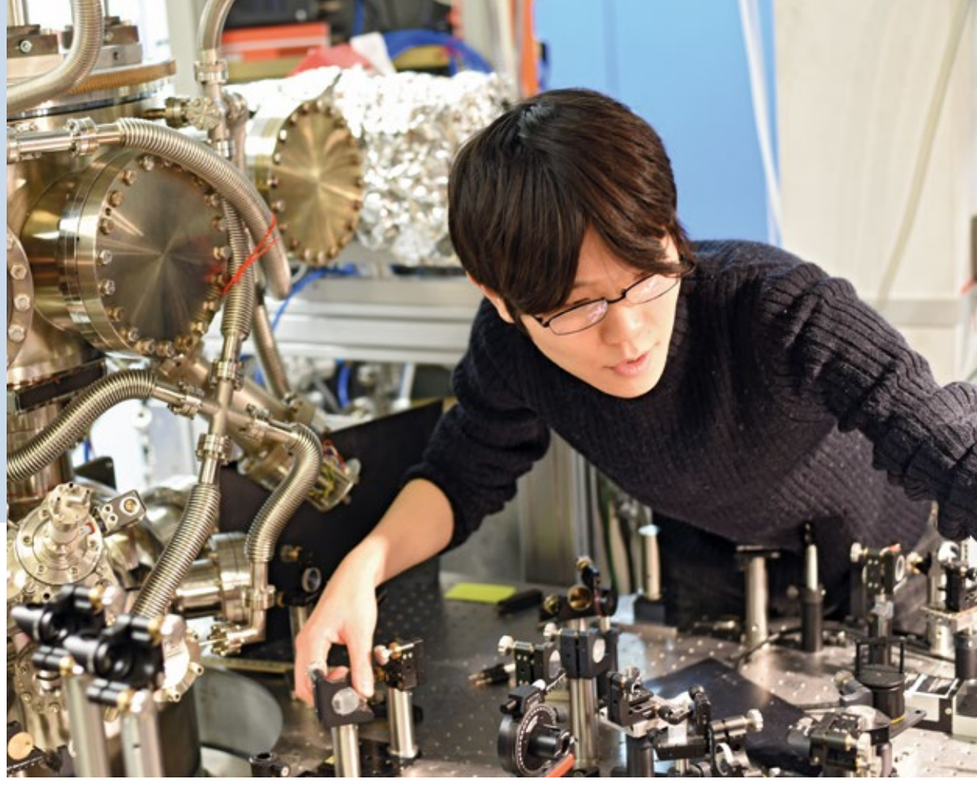
Laser spectroscopy is traditionally strong in Marburg. In SFB 1083, several working groups have successfully transferred their methodology to internal interfaces. Large investments were made in equipment for these experiments during the SFB's first funding period. It enables the groups to investigate the dynamics of electronic excitations and charge transfer processes at interfaces with femtosecond time resolution.

Of key importance for the SFB initiative has been the commissioning of the **scanning transmission electon microscope (STEM)** in 2012 and the subsequent investment for STEM sample preparation at the Materials Sciences Center (Wissenschaftliches Zentrum für Materialwissenschaften, WZMW) of the Philipps-Universität Marburg. The double-Cs corrected STEM can examine many solid/solid interfaces with atomic resolution.



The possibilities of photoelectron spectroscopy were significantly expanded in the first funding period with the construction of a high-laser harmonics source and again in the second funding period with a special photoemission electron microscope. These developments allow for **time-resolved photoemission tomography** and two-dimensional band mapping of surfaces and interfaces.



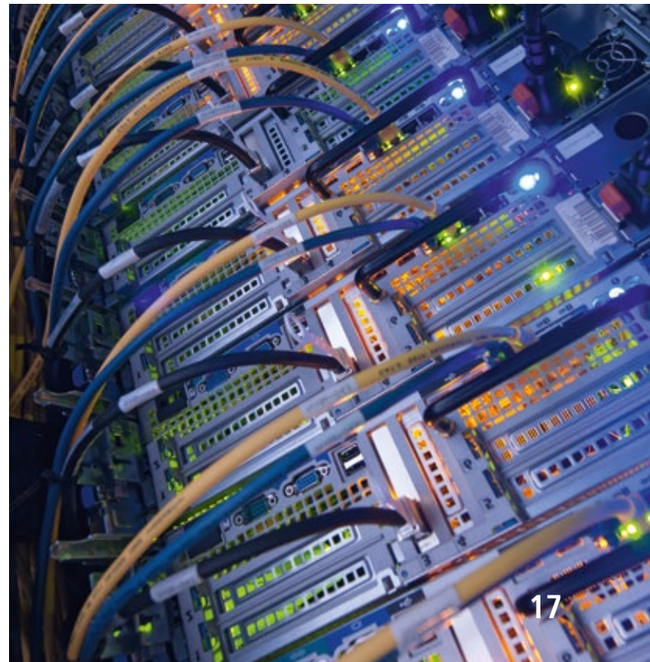


Complementary to laser-based photoelectron spectroscopy is the excitation with X-rays as it can access core levels and provide element-specific structural information. Hard-X-ray photoelectron spectroscopy (HAXPES) is able to probe interfaces buried below hundreds of atomic layers. Three working groups of SFB 1083 regularly have beam times at the **Berlin electron synchrotron BESSY II** and at the **British synchrotron Diamond** near Oxford.

Further basic equipment in SFB 1083 include **X-ray diffractometers** and **nuclear magnetic resonance (NMR) spectrometers** to determine the composition of newly synthesized compounds. Semiconductor heterostructures are grown by **metal organic vapor phase epitaxy (MOVPE)**. Many experiments at the interfaces are carried out in ultra-high vacuum (UHV), as this allows the best control of the sample parameters.

Theorists in SFB 1083, of course, require a wide range of computing power, depending on the problem at hand, ranging from the university's computing cluster to the national **high-performance computing centers**.

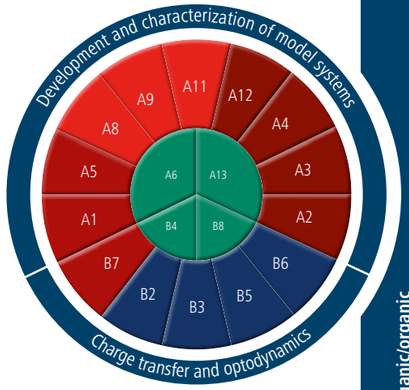
Last but not least, SFB 1083 benefits from a major investment (114 Mio EUR) of the state of Hesse in a new building for the chemistry department in Marburg in the framework of its HEUREKA programme.



Project Overview

As of 2019, SFB 1083 consists of 18 research projects listed below, as well as a public relations and a coordination project. Philipps-Universität Marburg is home to 15 projects, with Justus-Liebig-Universität Gießen (A8, B2), Forschungszentrum Jülich (A12) and Westfälische Wilhelms-Universität Münster (A13) as external partners.

	Principal Investigators		Project Title
A1	Prof. Dr. Wolfgang Stolz		**Metal organic vapour phase epitaxy of semiconductor heterostructures and interfaces**
A2	Prof. Dr. Gregor Witte		**Inorganic/organic and organic/organic interfaces: structure and charge transport**
A3	Prof. Dr. Peter Jakob		**Organic heterolayer interfaces: structure and vibrational excitations**
A4	Prof. Dr. Michael Gottfried Dr. Martin Schmid		**Reactivity, energetics and structure of buried organic/metal interfaces**
A5	Prof. Dr. Kerstin Volz		**Atomically resolved structure of solid/solid interfaces**
A6	PD Dr. Ralf Tonner		**Unified density functional description of bonding and interactions at inorganic/organic interfaces**
A8	Prof. Dr. Ulrich Koert Prof. Dr. Michael Dürr (Gießen)		**Organic molecular building blocks for the synthesis of internal interfaces**
A9	Prof. Dr. Stefanie Dehnen		**Synthesis and properties of molecular inorganic/inorganic/organic multilayer clusters**
A11	Dr. Johanna Heine		**Bismuth(III)iodide as a 2D material for hybrid compounds**
A12	Prof. Dr. Frank S. Tautz, Dr. François C. Bocquet, Prof. Dr. Christian Kumpf	(Jülich)	**Structure and phonons of hetero-epitaxial stacks of weakly interacting 2D materials and molecular layers**
A13	Prof. Dr. Michael Rohlfing (Münster)		**Theory of electronic interface states in weakly bound heterostructures**
B2	Prof. Dr. Sangam Chatterjee (Gießen)		**Ultrafast spectroscopy and control of excitations across internal interfaces**
B3	Prof. Dr. Martin Koch Prof. Dr. Wolfram Heimbrodt		**THz- and time-resolved optical spectroscopy of buried interfaces**
B4	Prof. Dr. Stephan W. Koch		**Microscopic theory of optical excitations in interface-dominated material systems**
B5	Prof. Dr. Ulrich Höfer Dr. Gerson Mette		**Time-resolved nonlinear optical spectroscopy at semiconductor interfaces**
B6	Prof. Dr. Ulrich Höfer Dr. Robert Wallauer		**Time-resolved two-photon photoemission studies of interface electron and exciton dynamics**
B7	Prof. Dr. Wolfgang Stolz Prof. Dr. Stephan W. Koch		**Interface-dominated semiconductor laser structures**
B8	Prof. Dr. Robert Berger		**Quantum chemistry for molecular vibrational and electronic transitions at organic interfaces**



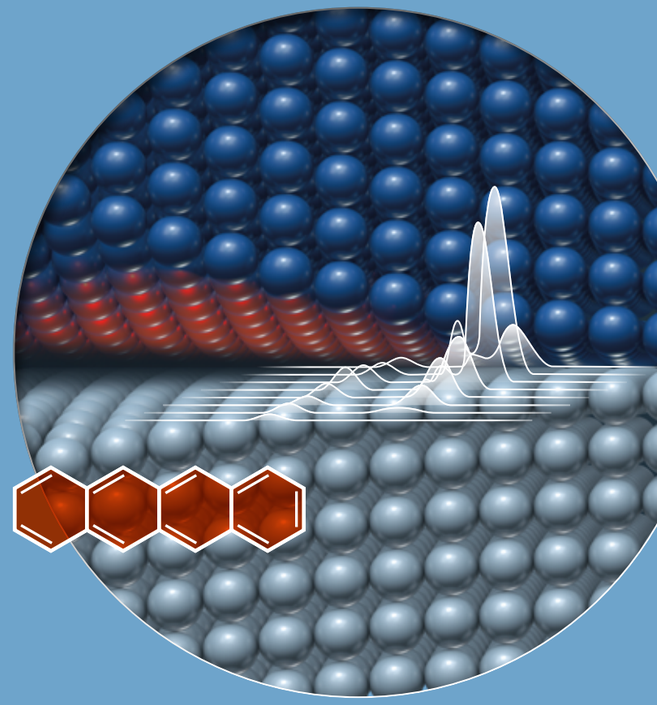
- semiconductor physics
- chemical synthesis
- surface science
- laser-spectroscopy
- theory/modelling

Spokesman:
Prof. Dr. Ulrich Höfer

Managing Board:
Prof. Dr. Kerstin Volz (vice-spokeswoman)
Prof. Dr. Michael Gottfried
Prof. Dr. Ulrich Koert
Prof. Dr. Stefan Tautz

Research Area	inorganic/organic	2D interfaces	metal/organic	organic/organic	inorganic/organic	chemical synthesis	epitaxial growth	structure analysis	optical spectroscopy	theory/modelling	
experimental physics	●						●	●	●		A1
experimental physics			●	●	●		●	●			A2
experimental physics			●	●			●	●	●		A3
physical chemistry			●				●	●			A4
experimental physics	●				●			●		●	A5
theoretical chemistry	●				●					●	A6
organic chemistry/ experimental physics				●	●	●	●	●			A8
inorganic chemistry		●			●	●		●			A9
inorganic chemistry		●			●	●	●				A11
experimental physics		●	●				●	●			A12
experimental physics		●	●							●	A13
experimental physics				●	●				●		B2
experimental physics	●								●		B3
theoretical physics	●	●								●	B4
experimental physics	●	●			●				●		B5
experimental physics		●	●	●	●		●		●		B6
experimental physics/ theoretical chemistry	●							●	●	●	B7
theoretical chemistry				●	●					●	B8

PUBLICATIONS



RESEARCH HIGHLIGHTS

Formation of an organic/metal interface state from a Shockley resonance

M.C.E. Galbraith, M. Marks, R. Tonner, U. Höfer

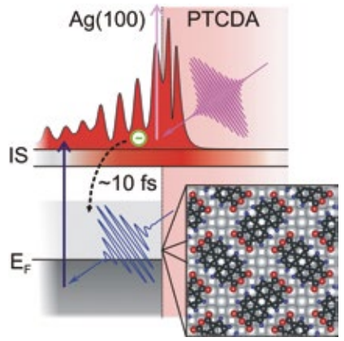
Journal of Physical Chemistry Letters **5**, 50 (2014)

An unoccupied organic/metal interface state is identified for PTCDA/Ag(100) by time-resolved two-photon-photoemission (2PPE) and further characterized by density functional theory. The interface state is located in the projected band gap of Ag(100) and has no direct counterpart on the clean metal surface nor in the molecular layer.

The coupling between the delocalized electron system of a metal and the orbital structure of organic molecules, and particularly the dynamical charge transfer between both entities, is one of the most challenging basic-physics problems of interface science. From the application point of view, well-defined interfaces of this type serve as models for electric contacts of organic semiconductor devices. Their operating frequency is still less than 10 MHz, and presently the limiting factor is the efficiency of charge carrier injection at the contacts. One strategy for improvement is to increase the contact area by nanostructuring. Complementary strategies may evolve from a detailed microscopic understanding of the mechanisms of the charge transfer.

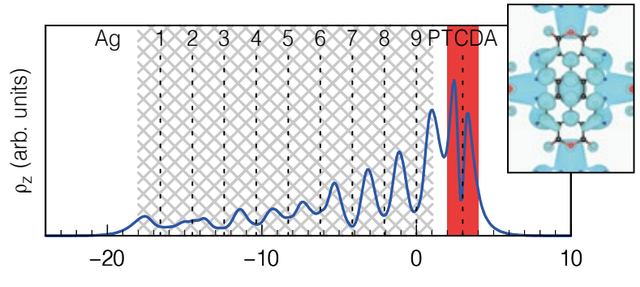
The authors identified an unoccupied electronic state at the interface between well ordered PTCDA layers and an Ag(100) single crystal. The state is found to have a dispersion parallel to the interface similar to a metallic band. At the same time, the spatial electron distribution above the molecular plane resembles that of a molecular orbital. The interface state is thus found to have very similar properties as the PTCDA/Ag(111) interface state (IS). This state, which was previously shown to be derived from the occupied Shockley state of the clean Ag(111) surface, is upshifted by the presence of the organic overlayer and becomes unoccupied.

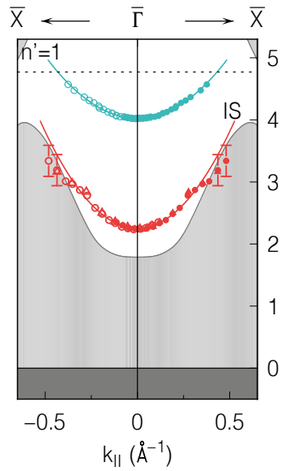
The results for Ag(100), where no such surface state exists, reveals that the existence of a Shockley state on the clean surface is not a prerequisite for the formation of interface states in the presence of organic overlayers. More generally, the IS originates from the symmetry break at the metal/organic interface. This gives rise to additional solutions of the Schrödinger equations that have no counterpart in the bulk metal or in the molecular layers. DFT calculations show that the IS probability density has its maximum between the metal substrate and the organic semiconductor. Similar to the Shockley states of clean metal surfaces, the IS probability density in the metal is that of an exponentially decaying Bloch state. In contrast to Shockley states, however, the IS is laterally strongly corrugated and has a hybrid organic/metal character. If the IS is located between the Fermi level of the metal and the organic LUMO it can thus efficiently mediate charge transfer between metal and organic semiconductor.



Excitation scheme of the 2PPE experiment. The first laser pulse excites electrons from occupied states of the substrate into the interface state (IS). Electrons from this transient population are then photoemitted by a second, time-delayed laser pulse and analyzed with respect to kinetic energy and emission angle. Reprinted with permission. Copyright 2014 American Chemical Society.

Probability density of the interface state (IS) perpendicular to the interface (main panel) and parallel to the interface (inset) for one PTCDA molecule of the surface unit cell. Reprinted with permission. Copyright 2014 American Chemical Society.





Dispersion of (IS) and image-potential state ($n' = 1$) plotted in the projected band structure. Occupied (unoccupied) bulk bands are shaded dark-gray (lightgray). Reprinted with permission. Copyright 2014 American Chemical Society.

Molecular packing determines singlet exciton fission in organic semiconductors

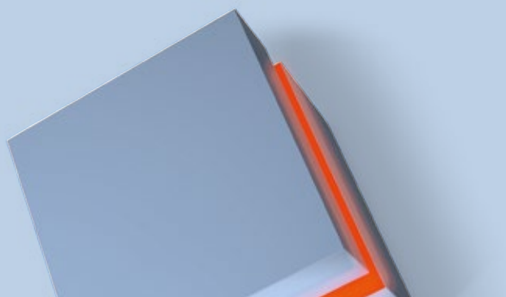
K. Kolata, T. Breuer, G. Witte, S. Chatterjee

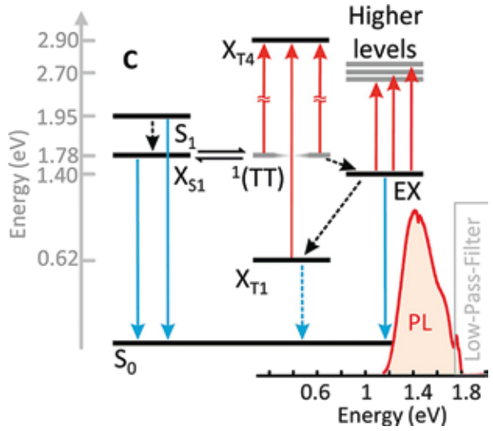
ACS Nano **8**, 7377 (2014)

The optimum performance of conventional photovoltaics is constrained by the Shockley-Queisser limit; about 30 % efficiency for silicon devices. Carrier multiplication by singlet-exciton fission in molecular semiconductors may enable enhanced efficiencies. Experiments shed light on carrier multiplication dynamics and reveal their relation to the molecular arrangement and consequently the intermolecular interaction in a model single crystalline system.

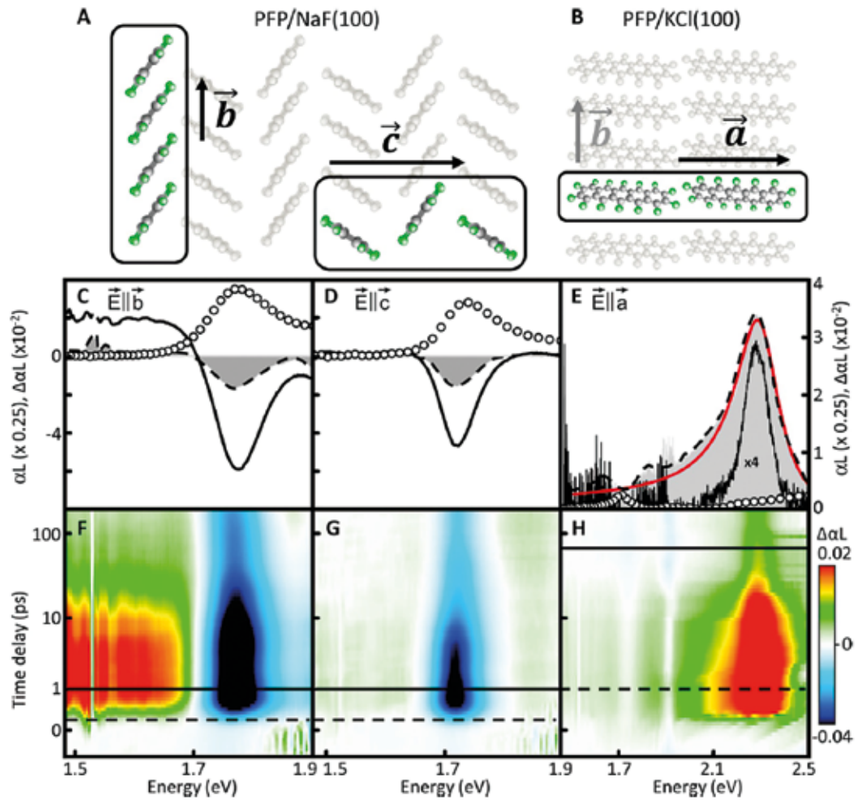
Singlet-exciton fission describes the conversion of a singlet exciton into two triplet excitons. In conventional photovoltaics, absorbed photons are converted into excitons that dissociate into a net current and excess energy is dissipated as heat. Carrier multiplication utilizes this excess energy to generate additional excited carriers. When the photon energy for generation of singlet excitons is about double or more than for triplet excitons, the excitation may be distributed to two triplets excitons. These are parity-forbidden for individual molecules and cannot be excited directly by individual photons. However, once triplet states are populated, they may contribute to charge generation and hence increase the quantum efficiency, eventually even above unity.

Experimental investigation by time- and polarization-resolved pump-probe measurements reveals a correlation between singlet-exciton fission and the molecular arrangement. Exploiting the specific epitaxial growth relations of the prototypical organic semiconductor perfluoropentacene ($C_{22}F_{14}$, PFP) on KCl(100) and NaF(100) substrates renders it possible to independently address all three crystal axes by linearly polarized light. The observed spectral signatures are highly anisotropic due to a strong uniaxial delocalization of the excitations which, in turn, leads to weakened molecular selection rules. The pronounced slip stacking of the molecules along the **b**-axis enhances the intermolecular coupling, accompanied by delocalization of singlet excitons and direct coupling to the correlated triplet pair $^1(TT)$. These findings significantly enhance the fundamental understanding of the relation between molecular arrangement and electronic response laying the foundation for future high-performance organic electro-optical devices.





Energy level scheme and underlying relaxation mechanisms implemented in a rate-equation model. Solid blue arrows represent radiative recombination; the dashed arrows non-radiative relaxation. Red arrows indicate induced absorption. The inset shows the photoluminescence spectrum of the sample. Reprinted with permission. Copyright 2014 American Chemical Society.



Correlation of packing scheme (A–B) and optical response (C–H) along all crystal axes. Linear absorption (circles) and corresponding differential absorption spectra at time delays of 300 fs (dashed) and 1 ps (solid), as well as induced absorption and a Fano fit (red) ($\vec{c}$-axis,) at 1 ps (dashed) and 90 ps (solid). The time evolution of the differential absorption are shown on a nonlinear time scale. Reprinted with permission. Copyright 2014 American Chemical Society.

Coherent terahertz control of vertical transport in semiconductor heterostructures

O. Vänskä, I. Tittonen, S.W. Koch, M. Kira

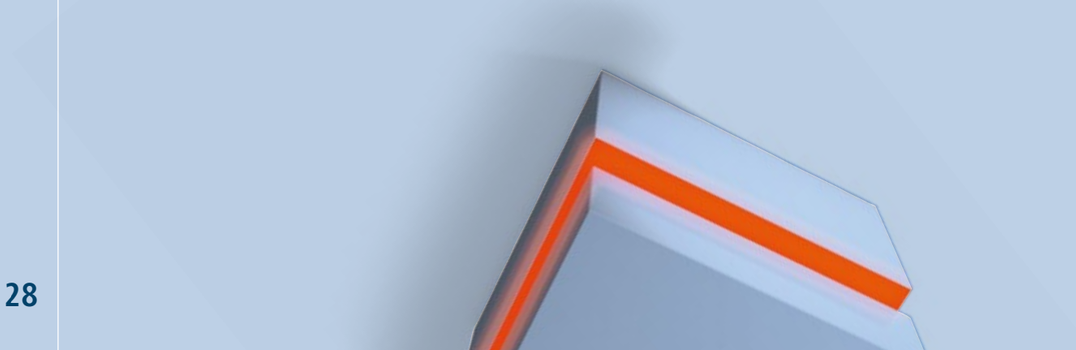
Physical Review Letters **114**, 116802 (2015)

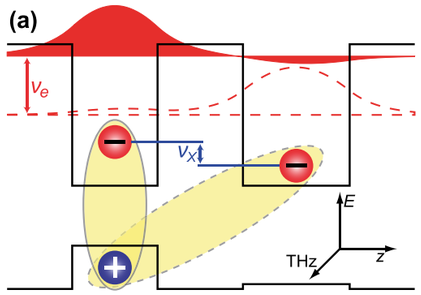
Vertical transport of currents across interfaces affects, e.g., solar cell functionality. A coherent-control protocols regulates selective transport of electrons, excitons, or pure two-particle correlations through semiconductor interfaces, as shown by a sequence of terahertz pulses applied to a double-quantum-well structure to initiate vertical excitation transfer between wells. Microscopic theory explains how this efficient and highly selective transfer works in the presence of unavoidable scattering and dephasing processes.

To study the fundamental physical properties of electronic excitation transport through interfaces between different semiconductor materials (vertical transport), a coherent control scheme was designed that makes it possible to selectively transfer charges, charge clusters, or even particular correlation properties through internal interfaces. In particular, vertical-transport protocols were developed that utilize sequences of terahertz (THz) pulses and can be applied to a wide variety of semiconductor heterostructures. These protocols were then applied to a model system, i.e., an optically excited, type-II double-quantum well (QW) structure. In this structure, the holes remain fixed in one of the wells while the electrons can be moved between QWs.

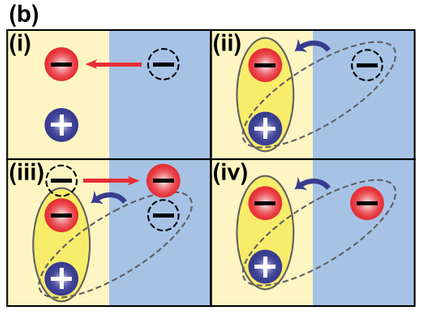
Systematic microscopic calculations show that a sequence of THz pulses can selectively transport either electron plasma or bound electron-hole pairs (excitons) through the interface. Through precise frequency tuning of the pulse sequence, it is not only possible to induce the selective electron or exciton transport, but also to design a protocol where purely exciton correlations are transferred across the internal interface. In other words, neither electrons nor excitons are transported in this case, only the correlations move through the double-QW interface. Importantly, the pure exciton-correlation transport is detectable by monitoring of the time-resolved photoluminescence.

The new protocols are significant in that their deviation from ideal operation is below 6 %, this suggests that they are sufficiently selective for characterization and utilization of interface properties in nanotechnology applications.





(a) Schematic configuration of the conduction- and valence-band edges of a double-QW structure with type-II band alignment. Here, the energetically lowest unbound electron-hole pair is indirect.



(b) Schematic presentation of protocols. While holes (blue spheres) remain in the left QW, electrons (red spheres) move through the interface, yielding (i) electron, (ii) exciton, and (iii) pure exciton-correlation transport. The dashed symbols denote the initial state and arrows identify the transitions; the net effect of protocol (iii) is summarized in frame (iv).
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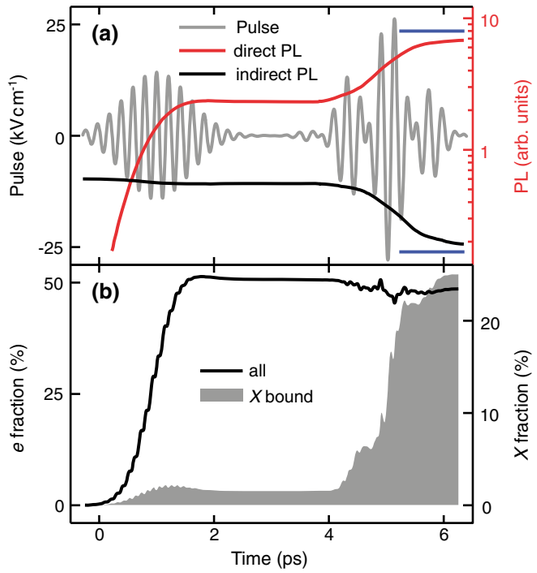

(a) A dual THz pulse (gray) is shown with the time-resolved luminescence at the direct (red) and indirect (black) exciton peak; vertical lines identify the luminescence levels reached when the second pulse is replaced with the pure exciton-transport protocol.

(b) Fraction of all (solid line) vs exciton-bound (shaded area) electrons as a function of time.
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Efficient syntheses of novel fluoro-substituted pentacenes and azapentacenes: molecular and solid-state properties

J. Schwaben, N. Münster, M. Klues, T. Breuer, P. Hofmann, K. Harms, G. Witte, U. Koert

Chemistry – A European Journal **21**, 13758 (2015)

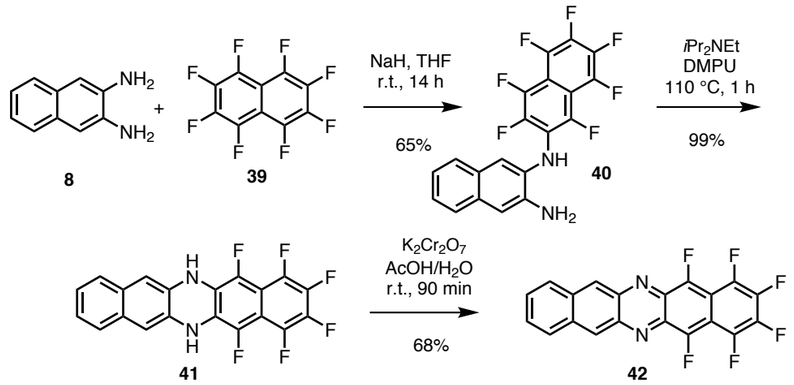
Pentacene is one prototype of a π-aromatic building block in organic electronics. It is marked by its ability to form structurally defined films and inorganic/organic interfaces. In addition, pentacene's stability can be increased by introducing nitrogen atoms into the π-aromatic system, while partial fluorination allows to introduce molecular dipole moments. With its highly-ordered and reproducible variability in the crystalline phase, pentacene and its derivates including azapentacene form important organic compounds.

In a combined experimental and computational approach, groups from chemistry and physics improved the synthesis of a range of novel partially fluorinated pentacene and azapentacene derivatives, at the same time providing full characterization of their properties ranging from crystal structure via optoelectronic properties to excitonic response.

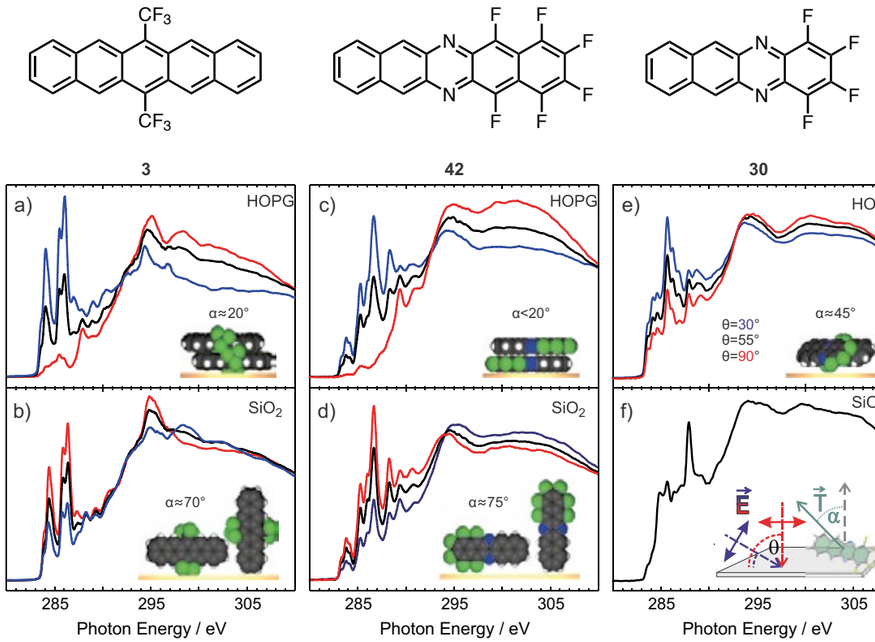
One example for an efficient synthesis is the synthetic route to diaza-hexafluoropentacene **42**. An intermolecular amination of the diamine **8** with perfluoronaphthalene **39** gives the diamine **40**. The subsequent intramolecular amination to produce the dihydrodiazapentacene **41** requires a careful adjustment of the base in order to prevent intermolecular side reactions. A final oxidation step then delivers the desired target compound **42**.

In addition to the crystal structure analysis and the comparison of their UV / Vis absorption spectra in solution and in the solid state, the thin film growth was investigated. Using X-ray absorption (NEXFAS) measurements to determine the molecular orientation from the dichroism of the π* resonances it is shown for compounds **3**, **30** and **42** that they adopt distinct recumbent and standing orientations on HOPG and SiO_2 substrates. Notably, the structural analysis of the asymmetrically fluorinated compound **42** exhibits an alternating pacing motif that is stabilized by its molecular dipole moment.

These novel fluoro-substituted pentacenes and azapentacenes are interesting candidates for various organoelectronic devices like, for example, organic-light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) and organic photovoltaics (OPVs).



Chemical synthesis of the diaza-hexafluoropentacene **42**.



Dichroic NEXAFS measurements of pentacene-type molecules **3**, **42** and **30** (top left to right) on HOPG (middle, highly oriented pyrolitic graphite) and SiO_2 (bottom) substrates. Inset pictures illustrate schematically the derived molecular orientation. (f) $\theta = 55°$ spectrum for compound 30 on SiO_2. Inset indicates definition of different angles.

Binding energy and dissociation barrier: experimental determination of the key parameters of the potential energy curve of diethyl ether on Si(001)

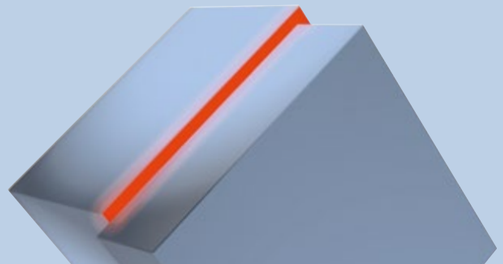
M. Reutzel, M.A. Lipponer, M. Dürr, U. Höfer

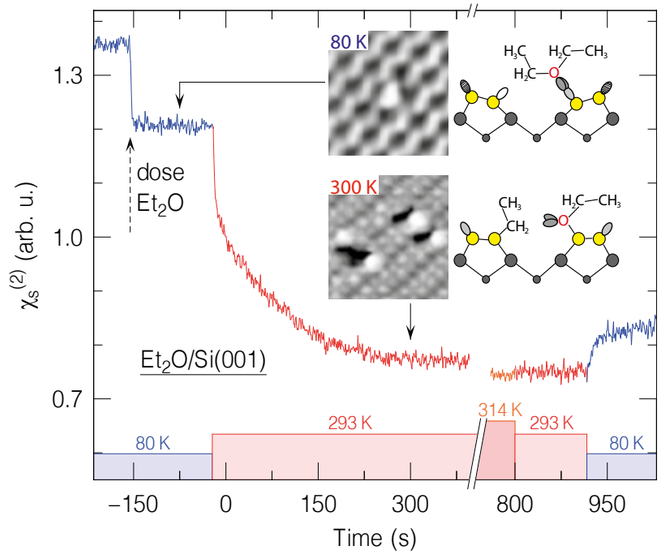
Journal of Physical Chemistry Letters **6**, 3971 (2015)

Following surface reactions in real time – optical second harmonic generation provides direct access to the kinetics of surface reactions of organic molecules on silicon.

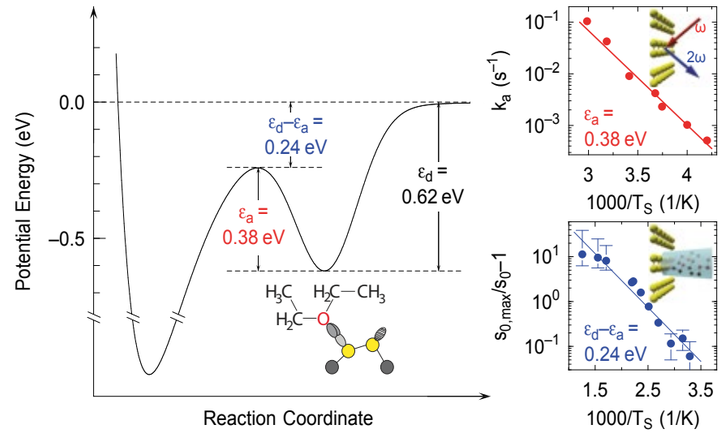
The adsorption of gas phase molecules on solid surfaces can be often decomposed into an initial adsorption step of the intact molecules and further reaction of these molecules on the surface. The latter reaction step can be very complex; in the case of organic molecules on silicon surfaces, it typically determines the final products. A precise understanding of the respective reaction kinetics is thus important for the control of such surface reactions. However, it is often difficult to monitor the kinetics of these surface reactions,as on the one hand, the probe has to be sensitive to the chemical changes on the surface, and on the other hand, it has to be fast enough in order to follow the respective chemical changes in real-time.

Physicists from Marburg and Gießen have thus developed a new approach for monitoring these surface reactions. They applied optical second harmonic generation (SHG) which can be very sensitive to chemical changes on the surface and therefore allow observation of the reaction kinetics in real-time over a wide range of time scales. With these measurements, ether cleavage of diethyl ether on Si(001) was studied in detail. For the first time, both the binding energy of an intermediate state and the respective conversion barrier into the final state were determined in a consistent measurement. As these are the two main parameters of the potential energy curve of such systems, they are also the basis for the controlled functionalization of semiconductor surfaces with organic molecules. Precise knowledge of these parameters can thus help to improve the quality of inorganic/organic interfaces and organic multilayers grown on these interfaces.





Optical second harmonic signal from Si(001) covered with a few percent of a monolayer of diethyl ether. When heating the sample (red part of the signal trace), the slow drop of the signal indicates ether cleavage on Si(001) and the kinetics of the reaction can be followed in real time. Reprinted with permission. Copyright 2015 American Chemical Society.



Measurement of the reaction kinetics by means of optical second harmonic generation allows for the determination of the reaction barrier ε_a for ether cleavage on Si(001). In combination with molecular beam techniques, the binding energy ε_d of the involved datively bound intermediate can also be determined. Reprinted with permission. Copyright 2015 American Chemical Society.

Synthesis of crystalline chalcogenides in ionic liquids

S. Santner, J. Heine, S. Dehnen

Angewandte Chemie – International Edition **55**, 876 (2016)

Crystalline chalcogenides may form dense solid-state structures, molecular cluster arrangements and highly porose networks. This diversity comes with interesting properties like semi-/photo-conductivity, ion transport capability, molecular trapping potential, chemical and catalytic activity. New types of chalcogenides and ways of contacting them to other materials or supports are therefore much sought.

Interest in novel chalcogenides drives synthesis strategies towards lower temperatures and better reaction control. Ionic liquids (ILs) can provide a tailorable designer-like medium for materials synthesis. ILs are salt-like compounds, which melt below 100 °C. Syntheses of crystalline chalcogenides under "ionothermal" conditions are very popular. Such reactions are carried out in sealed ampoules at moderate temperatures (up to 180 °C). Fine-tuning of reaction parameters allows access to compounds usually not available via traditional synthetic routes. While elevated temperatures mostly promote the formation of network compounds with extended anionic substructures, ionothermal approaches also allow for the formation of molecular, nanostructured subunits.

Synthesis of crystalline chalcogenido metalates based on binary and ternary molecular anions is advantageous as they are better soluble/dispersible. These anions form saltlike structures in the crystal, with mono-disperse, nanostructures anions besides ionic liquid cations. The challenge is to find conditions which suppress extended network formation. Molecular structures formed under ionothermal conditions can be exceptional, for example:

(1) $[Ge_{24}Sn_{36}Se_{132}]^{24-}$, the largest main group element anion, crystallizes in a variety of salts with different IL cations, which are capable of I_2 molecule take-up and heterolytic I-I bond cleavage.

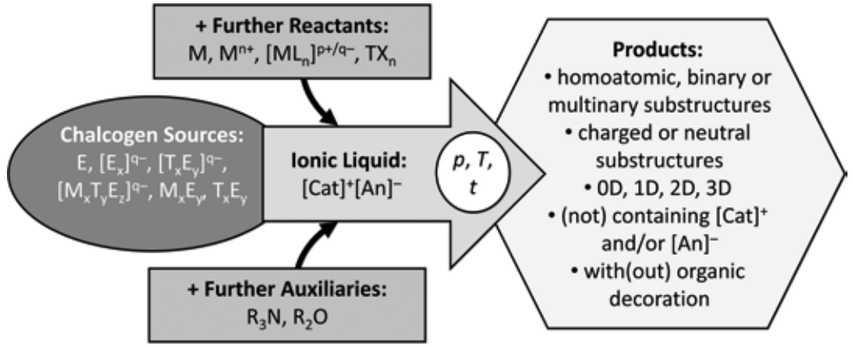
(2) $[Hg_8Te_{16}]^{8-}$, the tellurido mercurate anion, resembles the heaviest known topological analog of organic porphyrin. It crystallizes in lamellar salt structures with imidazolium-based IL counterions marked by very long alkyl chains. The so-formed double-layer structures are held together by van-der-Waals interactions only. They are thus subject to exfoliation and transfer to a solid support.

(C. Donsbach, K. Reiter, D. Sundholm, F. Weigend, S. Dehnen, Angew. Chem. Int. Ed. **57**, 8770 (2018))

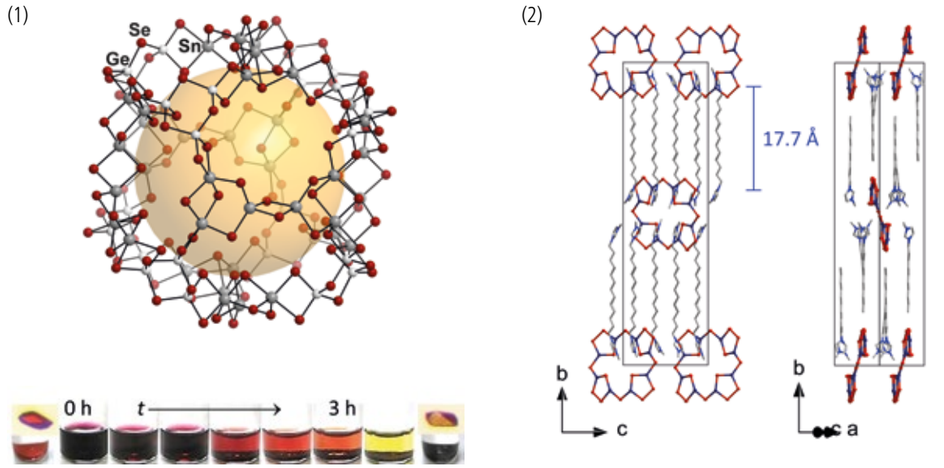
(3) $[Sn_{10}S_{16}O_4(SMe)_4]^{4-}$, a selectively alkylated chalcogenido metalate anion, results from methylation by the imidazolium cation of the IL "solvent". The very weak nucleophilicity of chalcogenido metalate clusters prohibits alkylation under common conditions with common reagents. Moreover, use of the relatively benign IL outperforms the use of toxic alkylation reagents. As the organic groups reduce the anionic charge, deposition of these clusters on uncharged or slightly polar surfaces comes into sight.

(B. Peters, S. Santner, C. Donsbach, P. Völpel, B. Smarsly, S. Dehnen, Chem. Sci. **10**, 5211 (2019))

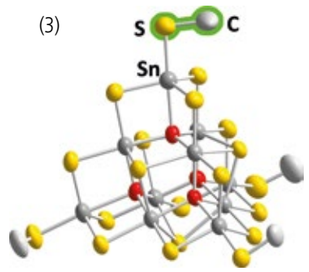
In summary, the uncommon nanostructured compounds obtained by ionotherm reactions have the potential of allowing controlled interaction with other solid materials via shared interfaces.



Schematic outline of the synthetic approach for the formation of crystalline chalcogen compounds in ionic liquids, indicating all parameters that can be varied. The auxiliaries need not to be part of the desired products; they instead help to trigger network formation or destruction. $[Cat]^+$ = cation, $[An]^-$ = anion. Copyright 2016 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.



Three examples of crystalline chalcogenido metalates formed under ionothermal conditions: (1) The "zeoball" anion $[Ge_{24}Sn_{36}Se_{132}]^{24-}$, with spherical shape and large cavity (yellow), and illustration of the I–I bond activation capability under formation of I_3^-. Copyright 2016 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
(2) Crystal structure section of the $[Hg_{18}Te_{16}]^{8-}$-salt with long-chain IL cations (blue and grey wires) in different orientations. Copyright 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
(3) Molecular structure of the cluster anion $[Sn_{10}S_{16}O_4(SMe)_4]^{4-}$, the first example of a chalcogenido metalate anion, selectively alkylated at the chalcogenide corners post-synthetically (B. Peters et al., Chem. Sci. **10**. 5211 (2019)).



Type-II vertical external-cavity surface-emitting laser with Watt level output powers at 1.2 µm

C. Möller, C. Fuchs, C. Berger, A. Ruiz-Perez, M. Koch, J. Hader, J.V. Moloney, S.W. Koch, W. Stolz

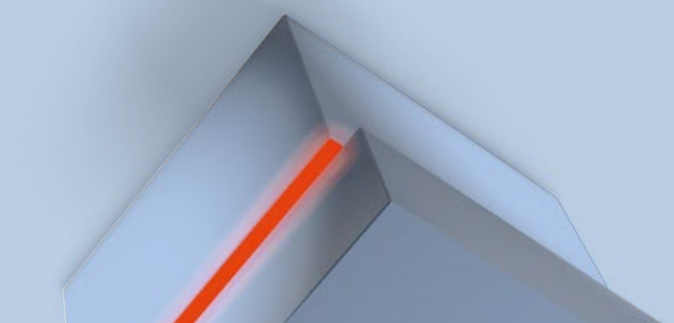
Applied Physics Letters **108**, 071102 (2016)

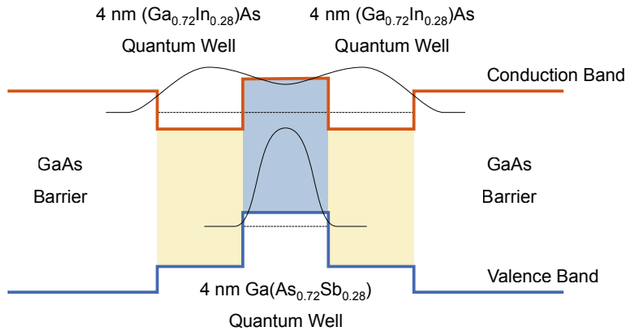
In a closed-loop cooperation of theoretical modelling and detailed experimental realization, novel interface-dominated type-II-W-quantum well heterostructures (QWH) are optimized for both edge- and surface-emitting semiconductor lasers, which are of great interest for telecommunication, optical data transfer and medical applications.

In comparison with type-I-QWH, a type-II-band alignment enables a more flexible band structure engineering in order to reduce intrinsic loss while the emission wavelength can be kept constant. Thus, such type-II-based lasers are promising candidates to surpass conventional type-I-lasers with respect to wavelength versatility and performance in the infrared wavelength regime. For this, their fundamental physical properties including interface characteristics need to be fully evaluated and explored both from the theoretical and experimental point-of-view.

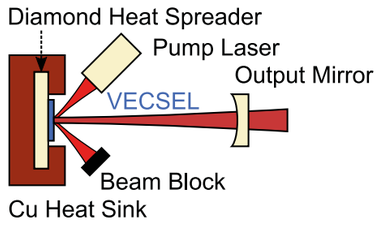
Detailed modelling of the optical characteristics, including the gain properties, of these type-II-W-QWH is achieved by fully microscopic theory. The resulting complex epitaxial III/V-compound semiconductor layer stack is realized by metal organic vapour phase epitaxy (MOVPE). The finished epitaxial layer stack is then mounted onto diamond heat spreaders and processed into a VECSEL active laser. The principle laser characteristics are analyzed from the laser properties of a simple linear resonator cavity, including an external output mirror. In joining forces three groups from Marburg contributed their expertise in theory, epitaxial realization and specific laser analysis, to iteratively optimize these VECSEL lasers.

The first successful realization of a VECSEL using this type-II-band alignment concept with optical output powers in the Watt level regime is shown. This success and also the realization of edge-emitting lasers in the 1.2 µm to 1.3 µm range, are the basis for exploration of additional combinations of material systems for longer emission wavelengths at 1.55 µm and beyond.

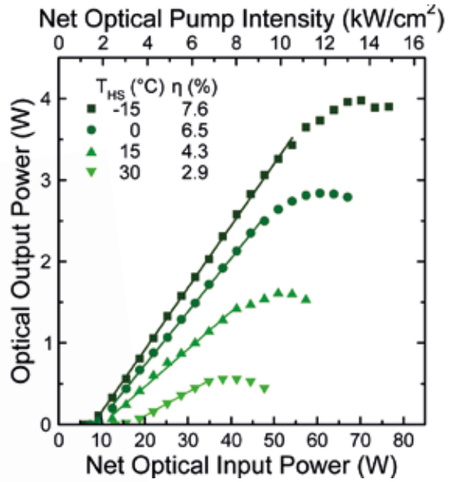




Schematic design of a type-II-W-quantum well heterostructure (QWH) in the (GaIn)As/Ga(AsSb)-based material system for laser applications.



Linear resonator structure of a vertical external-cavity surface-emitting laser (VECSEL).



Optical output characteristic of a type-II-W-QWH VECSEL as a function of heat sink temperature.
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Generation of transient photocurrents in the topological surface state of Sb_2Te_3 by direct optical excitation with mid-infrared pulses

K. Kuroda, J. Reimann, J. Güdde, U. Höfer

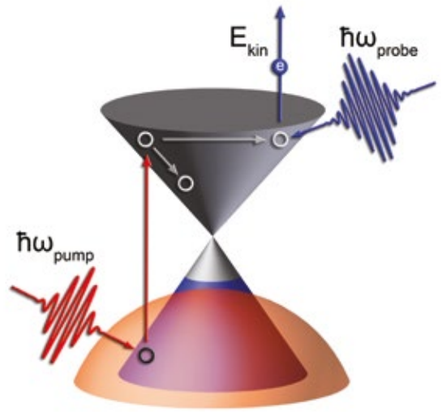
Physical Review Letters **116**, 076801 (2016)

The Dirac cone surface states of three-dimensional topological insulators are characterized by a chiral spin texture in k-space with the electron spin locked to its parallel momentum. It is demonstrated by means of time- and angle-resolved two-photon photoemission (2PPE) that pulsed laser excitation of such a topological surface state (TSS) in Sb_2Te_3 offers the possibility to create and control spin-polarized electrical surface currents on ultrafast timescales.

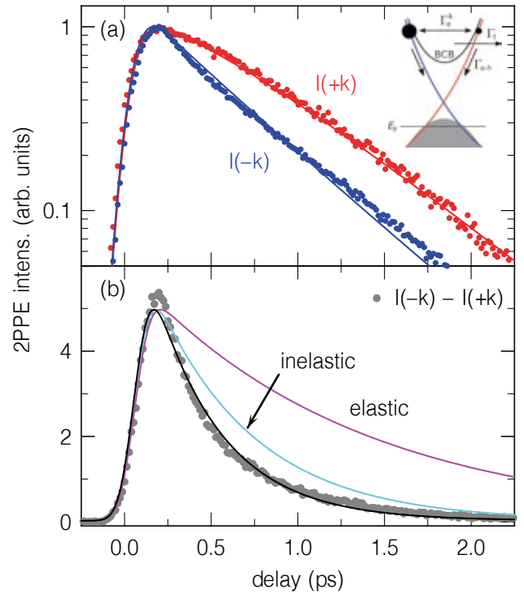
Topological insulators like Bi_2Se_3, Bi_2Te_3, Sb_2Te_3 and related materials have a band gap like ordinary semiconductors. The bulk of these materials is thus insulating at low temperatures. The electronic structure of the surfaces of these materials, however, is characterized by two-dimensional metallic states, so-called topological surface states (TSS) which have the form of Dirac cones at the Gamma point. In the TSS, the electron spin is locked to the parallel momentum. This chiral spin texture as well as the protection of the TSS by time-reversal symmetry makes topological insulators very promising for spintronic applications.

Kuroda and coworkers employed mid-infrared (MIR) pulses with photon energies below the bulk band gap in order to directly excite electrons from the occupied into the unoccupied part of the TSS. With this pump scheme across the Dirac point, they were able to create a pronounced asymmetry of the transient TSS population in momentum space which corresponds to a spin-polarized photocurrent in real space. Time-delayed photo-emission out of the TSS allowed for detailed investigations of the microscopic scattering processes leading to the decay of the surface currents. The elastic scattering time of 2.5 ps deduced for Sb_2Te_3 corresponds to a mean-fee path of 0.6 µm. These values exceed those of electrons on metal surfaces by two orders of magnitude. The results provide clear experimental evidence that the TSS electrons are effectively protected from back scattering by phonons and non-magnetic impurities.

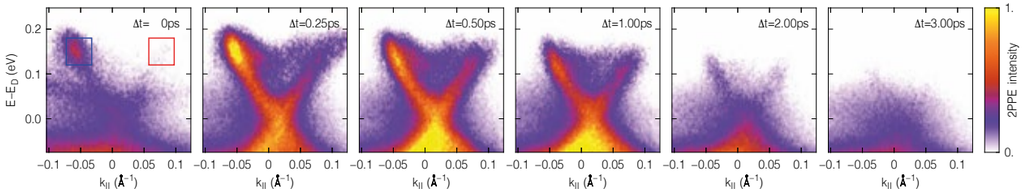
The discovery of optical coupling between the occupied and the unoccupied part of the TSS across the Dirac point promises important advantages of photoexcitation by mid-IR pulses for spintronic applications. The novel direct excitation scheme permits the ultrafast generation of an unbalanced transient electron population in momentum space. Since this corresponds to a photoexcited electric current the work thus opens a pathway for a coherent optical control of spin-polarized electrical currents.



Scheme of the experiment.



Normalized 2PPE intensity of the transient population in the Dirac cone at opposite parallel momenta, Intensity difference, and contributions of elastic momentum scattering and inelastic decay to the current decay. Reprinted with Permission. Copyright 2017 SPIE.



Angle-resolved 2PPE spectra for different time delays between the mid-IR pump and the UV probe pulses. For a video see www.physik.uni-marburg.de/of/publications/abstracts/kuroda17spie.html. Reprinted with Permission. Copyright 2017 SPIE.

Electron–vibron coupling at metal–organic interfaces from theory and experiment

P. Rosenow, P. Jakob, R. Tonner

Journal of Physical Chemistry Letters **7**, 1422 (2016)

Metal-organic interfaces are essential elements influencing the performance of molecular electronics applications like light-emitting devices or field-effect transistors. Here electronic excitations via charge-transfer excitons often play a key role. The formation mechanisms of these excitons via electron-hole pair (EHP) formation at the interface thus need to be understood. The coupling of EHP to adsorbate vibrations (electron-vibron coupling) is one way to induce an interfacial dynamical charge transfer (IDCT), which delivers key information about the electronic structure at the interface. IDCT induced by an orbital dipping in and out of the Fermi sea has been suggested for small molecules on metal surfaces.

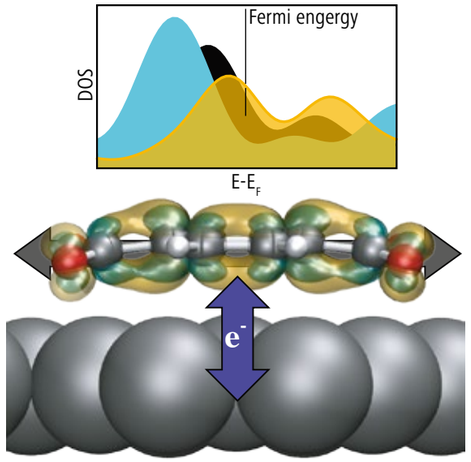
This effect, where vibrational modes become infrared active due to electron flow across the interface, has been previously described using theoretical reasoning and heuristic models. However, the new study provides the first proof and quantitative examination thereof based on first-principles calculations. Thus, the findings provide an important insight into a key electronic property of interfaces between organic molecules and coinage metal surfaces.

The effect of electron-vibron coupling is observed for molecular adsorbates, when a molecular orbital is partially filled upon adsorption (static charge transfer), such that its occupation changes dynamically during certain vibrations with respect to the Fermi level of the surface (dynamical charge transfer). This leads to an electron flow between metal and adsorbate, giving rise to an oscillating dipole moment perpendicular to the surface. This fulfils the selection rule for infrared activity.

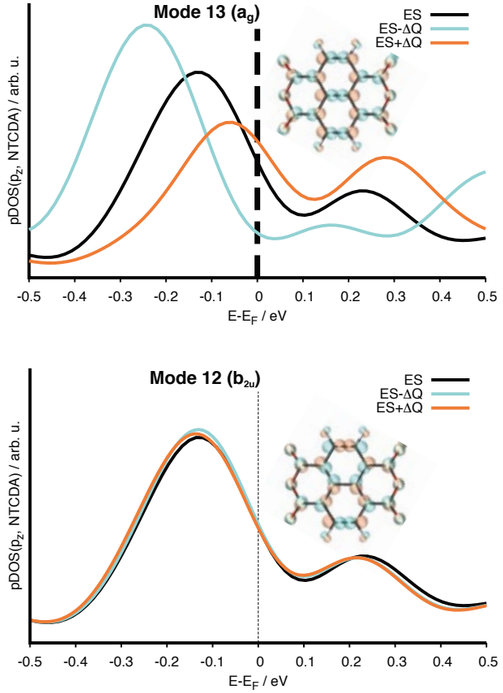
1,4,5,8-Naphthalenetetracarboxylic dianhydride (NTCDA), a common model compound for an important class of organic semiconductors, adsorbs on the Ag(111) surface by accepting metal electrons in the lowest unoccupied molecular orbital (LUMO), thus fulfilling the above requirement. Molecular vibrations with a specific symmetry can usually not be observed in infrared spectroscopy in the gas phase. However, strong signals were observed in the experimental spectrum of the molecule adsorbed on the surface for the very same modes. By theoretical investigations it could be proven that this is due to strong IDCT effects.

By studying the projected density of p-symmetric electronic states, the observation was verified with first-principles calculations and the effect was quantified with partial charge analysis. An excellent correlation between charge transfer and infrared intensity for the fully symmetric vibrational modes was found.

The general approach derived will facilitate the analysis of other relevant metal-organic interfaces with similar matching of energy levels in the future. On the basis of the thus obtained improved understanding, fine-tuning of the atomic and electronic structure for these types of interfaces becomes feasible.



Interface dynamical charge transfer (IDCT) for a metal-organic interface and the signature created in the density of states (DOS). Reprinted with permission. Copyright 2016 American Chemical Society.



Total symmetric modes show a significant change in charge density (top) while modes with other symmetry (bottom) do not show this phenomenon. Reprinted with permission. Copyright 2016 American Chemical Society.

Pyramidal structure formation at the interface between III/V semiconductors and silicon

A. Beyer, A. Stegmüller, J.O. Oelerich, K. Jandieri, K. Werner, G. Mette, W. Stolz, S.D. Baranovskii, R. Tonner, K. Volz

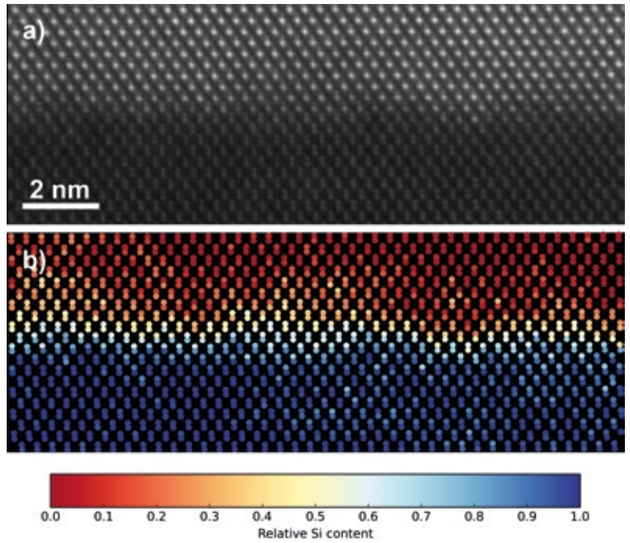
Chemistry of Materials **28**, 3265 (2016)

Modern semiconductor devices, as found in cell phones, personal computers or solar cells are commonly based on silicon. However, the last years have shown that computing speed ceases to experience significant increase and efficiency gain for conventional solar cells is slowing as silicon-based technique reaches several fundamental limits (e.g., the tunneling of electrons through nanometer-sized device structures). To overcome these physical limits, silicon can be coated with other materials. III/V-semiconductors, which consist of elements of the 3rd and 5th group of the periodic table (group 13 and 15 in chemical science nomenclature), are well suited for this task. However, the combination of these two material classes holds several challenges: foremost is finding materials with the same lattice constant as silicon, since this leads to more stable devices.

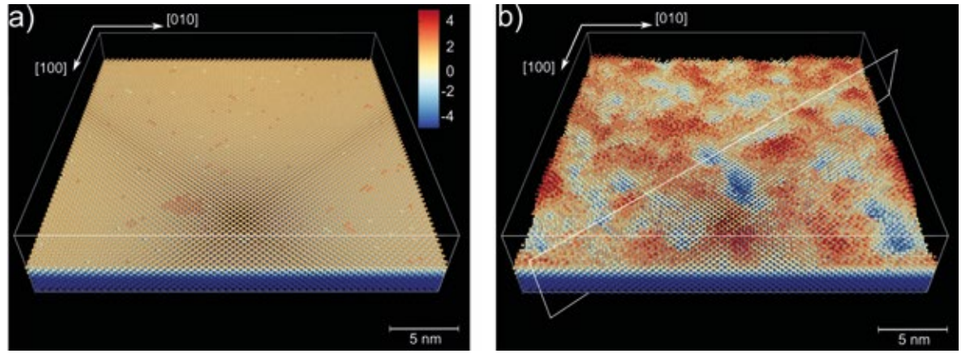
III/V-semiconductors with the same lattice constant as silicon have been observed. However, they still differ from silicon in other important properties, especially in their polarity, which may lead to defects forming at the interface between the two materials and the accumulation of undesired charges, which limit the functionality of the device.

To find a solution to this challenge, the model system of galliumphosphide (GaP) on Si was investigated by several groups in Marburg. State of the art aberration-corrected electron microscopy was used to determine the structure at the interface at unprecedented atomic resolution, revealing that the actual interface between GaP and Si is not perfectly flat but exhibits a distinct structure across several layers of intermixing. Quantitative modelling of the electron scattering process taking place within the microscope, showed that the interface between the silicon substrate and the III/V-semiconductor exhibits this pyramidal morphology despite the initial silicon surface clearly having been atomically flat prior to GaP growth.

This pyramidal interface morphology is an intrinsic feature of combining these two materials in a sense that this structure was observed in samples grown under markedly different conditions. Theoretical modelling taking kinetic and thermodynamic processes into account has helped to understand the processes leading to this structured interface. Density functional theory explains that the pyramidally shaped interface structure is energetically favorable over an abrupt flat interface as local charges are better compensated for in structured interfaces. Moreover, a kinetic driving force based on diffusion in the growth process was found, which results in the intermixing. In consequence, this structural formation at the interface appears to be a general feature which needs to be considered for all III/V materials grown on silicon. At the same time, the results gained promise to open up new possibilities for future intentional altering of the interface structure, opening up a pathway to increasing the efficiency of existing devices or even developing novel ones.



Atomically resolved STEM (scanning transmission electron microscopy) images of the GaP/Si interface region in [110] viewing direction (a). The occupancy of each atomic column with Si is plotted in (b). Reprinted with permission. Copyright 2016 American Chemical Society.



Silicon surfaces prior to and after GaP deposition as obtained from the KMC (Kinetic Monte Carlo) simulation. Similar to the experiment, the Si surface after Si deposition in the KMC simulation is atomically flat (a). After GaP deposition, a structured Si interface is obtained (b) (the Ga and P atoms are not shown in the picture for clarity), which exhibits a highly structured morphology, similar to the interface structure observed experimentally. Reprinted with permission. Copyright 2016 American Chemical Society.

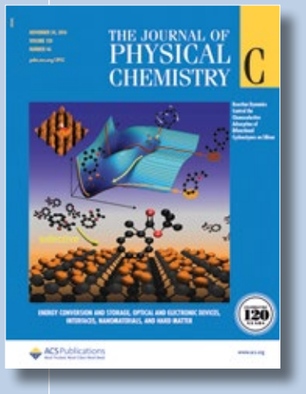
Chemoselective reactivity of bifunctional cyclooctynes on Si(001)

M. Reutzel, N. Münster, M.A. Lipponer, C. Länger, U. Höfer, U. Koert, M. Dürr

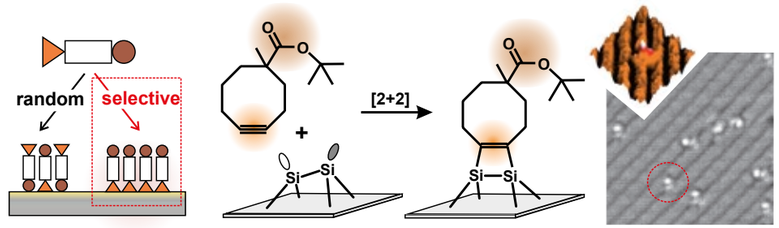
Journal of Physical Chemistry C **120**, 26284 (2016)

Controlled functionalization of semiconductor surfaces with organic molecules offers new perspectives in semiconductor technology ("More than Moore"). Chemoselective attachment of multifunctional organic molecules is the first fundamental process step for such a controlled organic functionalization of semiconductor surfaces. However, the high reactivity of pristine silicon surfaces, especially of the technologically most relevant Si(001) surface, has so far prohibited such a controlled organic functionalization of silicon: multifunctional molecules typically do not show chemical selectivity on Si surfaces, but are found with different functional groups attached.

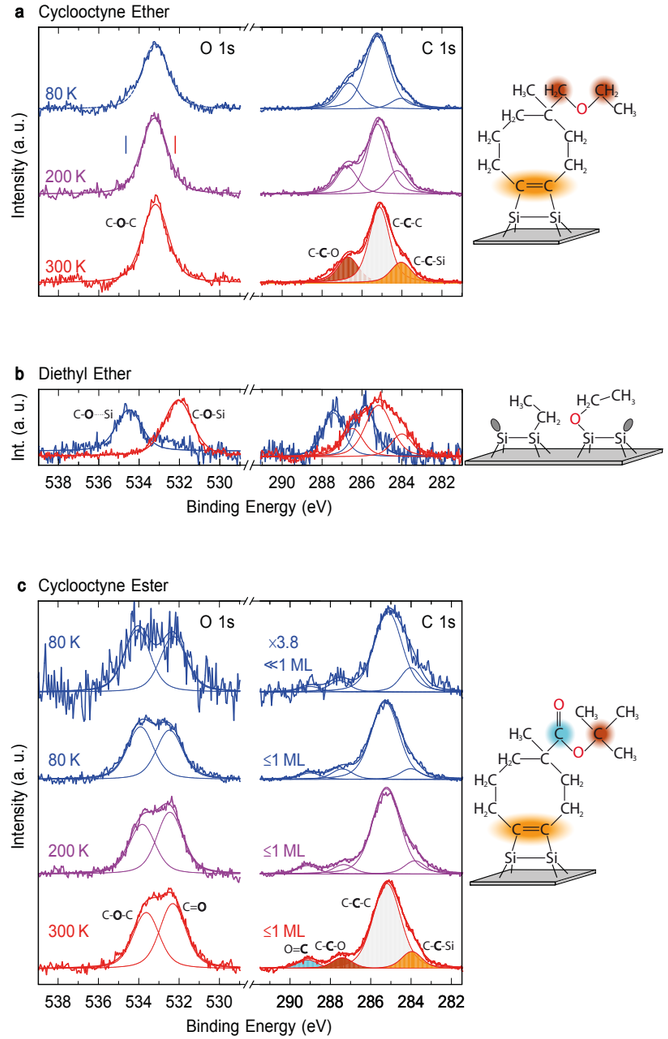
In a joint effort, chemists and physicists of SFB 1083 developed for the first time a general strategy for solving this problem: Using substituted cyclooctynes, they were able to obtain well-defined inorganic-organic interfaces on Si(001), with the bifunctional molecules being attached to the silicon surface solely via cyclooctyne's strained triple bond. The second functionality of the substituted cyclooctyne is thus available for further building up of complex molecular architectures, e.g., using organic click chemistry.



The strategy for the observed chemoselectivity is based on the distinctly different adsorption dynamics of the separate functionalities: The strained triple bond of cyclooctyne adsorbs on silicon via a "direct" reaction channel. In contrast, almost all other organic functional groups adsorb on silicon via an "indirect" reaction channel, which makes them effectively unreactive in competition with the direct pathway of cyclooctyne's strained triple bond. As a consequence, the concept is largely independent on the nature of the second functional group, which can be chosen according to the further reaction schemes employed. The cyclooctyne layer thus forms a versatile interface between the silicon substrate and the world of organic chemistry; it can be the basis for a multitude of applications, e.g., the integration of optically active organic layers on silicon devices. The obtained structures are also of high interest for further studies of the electronic properties at organic/semiconductor interfaces within SFB 1083.



Interface between semiconductor technology and organic chemistry: cyclooctyne selectively attaches to the silicon surface via cyclooctyne's strained triple bond. Reprinted with permission. Copyright 2016 American Chemical Society.



XPS results unambiguously demonstrate the chemoselective adsorption of both, cyclooctyne ether and cyclooctyne ester, on Si(001) via the strained triple bond of cyclooctyne. Reprinted with permission. Copyright 2016 American Chemical Society.

Intervalley scattering in MoS_2 imaged by two-photon photoemission with a high-harmonic probe

R. Wallauer, N. Armbrust, J. Reimann, J. Güdde, U. Höfer

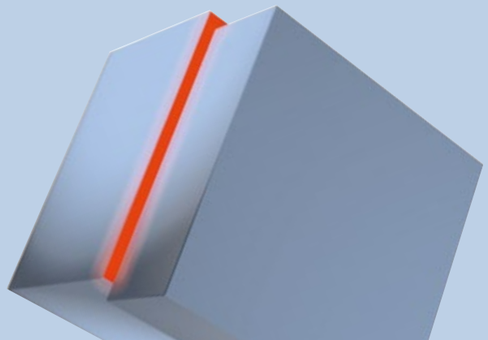
Applied Physics Letters **109**, 162102 (2016)

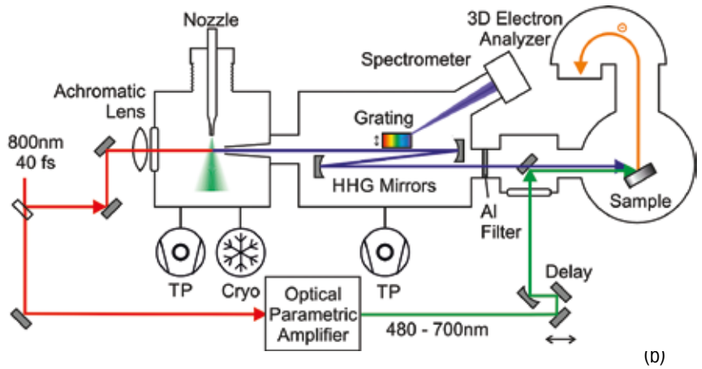
A new experimental setup for time-resolved two-photon photoemission (2PPE) is reported. The method, which combines femtosecond pump-probe techniques with photoelectron spectroscopy, makes it possible to map the dynamics of electron transfer processes at surfaces and interfaces directly in momentum space.

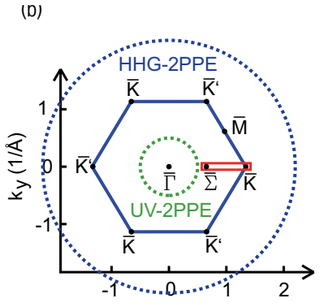
The new experiment combines a high-harmonic generation (HHG) light source, developed and built in Marburg, with a state-of-the-art 3D hemispherical electron analyzer (VG Scienta DA30). The analyzer can measure electron energies as a function of both parallel momentum directions (k_x and k_y) without movement of the sample. The highest electron momentum accessible in photoemission, the so-called photoemission horizon, is directly related to the photon energy available. The high-harmonic source gives access to the full 2D Brillouin zone whereas conventional 2PPE setups are restricted to electrons near the Γ point.

The large parallel momenta, which become accessible with the new experiment, enable SFB 1083 to study electron dynamics at interfaces of many interesting new materials. Particularly, in the class of two-dimensional transition-metal dichalcogenides (TMDCs), most of the interesting electron dynamics take place at the boundary of the first Brillouin zone. Investigations of the intervalley scattering in the topmost layer of MoS_2, a prototypical TMDC, demonstrate this capability. Electrons excited at the K-point are found to scatter to the Σ-point in less than 50 fs by directly mapping the electron population in k-space as a function of time.

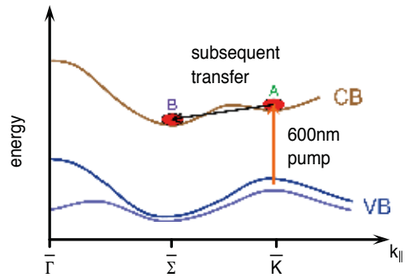
The new experiment opens up the possibility to study charge transfer and exciton formation with 2PPE in a variety of systems, most prominently van-der-Waals heterostructures, which are a combination of different single-layer TMDCs. In these systems, upon excitation, charge transfer excitons can form. Their formation and relaxation pathways can now be examined by a direct mapping technique in momentum space.



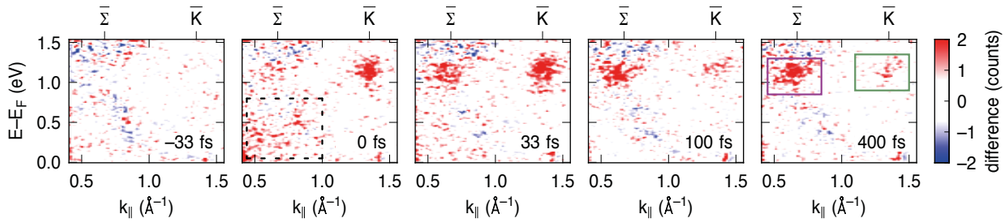




(a) Sketch of the experimental setup. (b) Brillouin zone of MoS_2 and photoemission horizon (dashed circles) for 2PPE with laser systems that use UV light as a probe (green dashed circle) and for HHG-based systems (blue dashed circle). Reproduced with the permission of AIP Publishing.



Pump-/Probe scheme with the excitation at $\bar{K}$ followed by the ultrafast transfer to $\bar{\Sigma}$ (left). In the delay series (below) the fast transfer to $\bar{\Sigma}$ can be observed, where the population appears within the first time step (center). A population remains visible at both high symmetry points over the observed delay range. Reproduced with the permission of AIP Publishing.



Model potential for the description of metal/organic interface states

N. Armbrust, F. Schiller, J. Güdde, U. Höfer

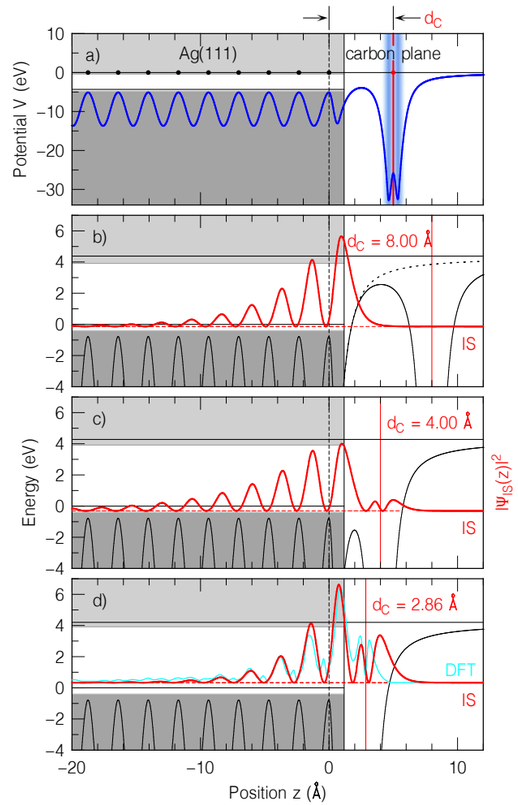
Scientific Reports **7**, 46561 (2017)

An analytical one-dimensional model potential predicts the energy position and the wave function overlap of metal/organic interface states. It explains how the energy of the interface state depends systematically on the bond distance between the carbon backbone of the adlayers and the metal. Comparison with numerous experimental results demonstrates the general applicability and robustness of the model.

Charge transfer at the interface between a metal and a layer of organic molecules plays a decisive role in the functionality of organic semiconductor devices and for future applications of molecular electronics. It depends crucially on the energy alignment and the wave function overlap of electronic states at such interfaces. Of particular interest for model studies are interface-specific electronic states like the ones observed for PTCDA and other π-conjugated organic molecular layers grown on Ag(111). These interface states originate from the Shockley surface state of the bare metal substrate. This state is upshifted due to the interaction with the molecular layer while hybridization of molecular and metallic states remains rather small in the region of the projected band gap of the metal.

In order to highlight the main physical mechanism for the formation of the delocalized interface state at organic/metal interfaces without the help of complex DFT calculations, Armbrust and coworkers propose a one-dimensional description by an analytical model potential. The choice of the potential is inspired by previous work on surface states of clean metals. It utilizes graphene as a universal representation of flat-lying adlayers of π-conjugated organic molecules. Unlike other, more adsorbate-specific model potentials used previously to describe interfacial electronic states, its main parameter is simply the distance of the carbon plane from the metal substrate.

The work shows that the same model potential not only predicts the energy of the interface state in various graphene/metal systems, but can be applied to a large class of flat-lying molecular layers with a similar π-π interaction as in graphene. The model calculation clearly illustrates how the interface state develops from the former Shockley-type surface state of the bare metal substrate with increasing interaction between the molecular film and the metal. By comparing the results with available experimental data for different organic molecules, the authors show that their model is able to describe the systematic dependence of the energy of the interface state on the bond distance between the carbon backbone and the metal with predictive power. Moreover, the model reveals how the wave function overlap of the interface state with both the bulk metal and the molecular overlayer depends on the carbon-metal distance.



One-dimensional model potential V(z) for a carbon layer on Ag(111) and the probability densities $|\Psi$ IS(z)$|^2$ of the interface state formed at differing metal-C distances (Reprinted with permission).

Energy shift of the interface state with respect to the energy of the former surface state on the bare metal as a function of the carbon-metal distance (Reprinted with permission).

Ethers on Si(001): a prime example for the common ground between surface science and molecular organic chemistry

L. Pecher, S. Laref, M. Paupach, R. Tonner

Angewandte Chemie – International Edition **56**, 15150 (2017)

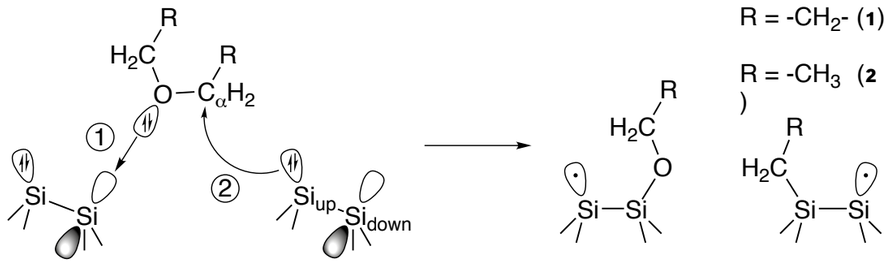
Material science and surface science are pushing forward the development of new technologies and electronic devices. More recently, organic molecules have begun to be used, e.g., in the construction of organic light-emitting devices (OLEDs) or the organic functionalization of semiconductors. Chemical expertise is indispensable in describing the underlying bonding and reactivity phenomena. Especially on semiconductor surfaces, where electronic states are more localized compared to delocalized states on metals, the surface often behaves like a molecular reagent and solution chemistry concepts can be very helpful in describing the system.

The Si(001) surface is a widely used substrate due to its relevance for application and its high reactivity arising from both nucleophilic and electrophilic surface atoms being present. Ethers show an unexpectedly rich reactivity at the surface, a result that sparked extensive experimental investigation. Spectroscopy revealed a datively bonded (DB) intermediate and subsequent regioselective C-O bond breaking with a sizeable barrier. The surface-induced bond cleavage was proposed to stem from σ^*(C-O) occupation in the DB state. These results render the system an ideal model for a theoretical approach.

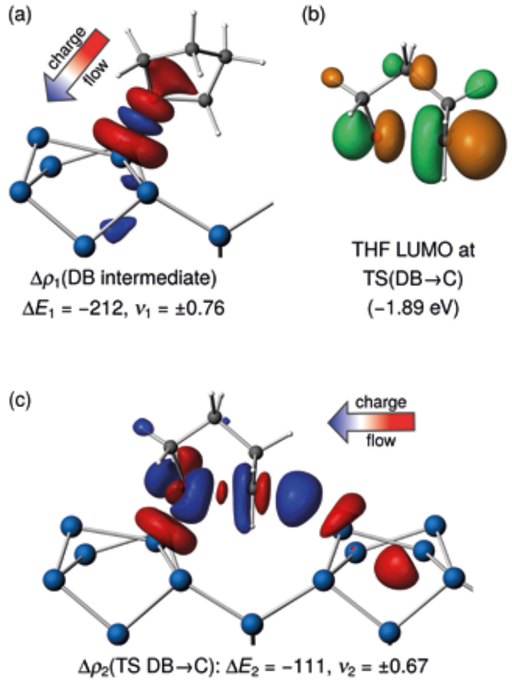
The well-known surface reconstruction of Si(001) sees the formation of buckled dimers with an electronic structure well approximated by an empty p orbital at the Lewis acidic Si_{down} dimer atom and a non-bonding electron pair at the Lewis basic and nucleophilic Si_{up} atom. Therefore, a mechanism analogous to the ether reaction known from molecular chemistry suggests itself: In the first step, a DB intermediate is formed between the oxygen and Si_{down} atoms while in the second step, any nearby nucleophilic Si_{up} atom can attack a C_α atom to form a covalent Si-C bond.

This mechanism was proven by a quantitative analysis of the electronic structure in the surface-adsorbate system. By a novel approach of decomposing the bonding energy into well-defined physical terms (periodic energy decomposition analysis, pEDA), the main features of the reaction could be highlighted. It turned out that the datively bonded intermediate shows donation of the σ- and π-type non-bonding electron pair into the formally empty surface state, thus explaining the high stability. The regioselective ether cleavage is then understood as following a reaction pathway that closely resembles the nucleophilic reaction (S_N2) known from textbook organic chemistry with bond-making and bond-breaking happening at the same time.

Thus, by quantitative electronic structure analysis the bonding, reactivity, and regioselectivity in this model system was proven to proceed very similarly to classical reactions of organic chemistry. This demonstrates that even under ultrahigh vacuum conditions on surfaces, which differ from the usual solvent-based conditions of chemistry, simple chemical concepts are applicable and allow prediction. The reported nucleophilic substitution reaction can be expected to occur with any molecule having a Lewis basic group and a nearby carbon atom that can be attacked. This establishes nucleophilic substitution as a common class of surface reaction on semiconductor surfaces.



Two-step reaction of ether molecules with the Si(001) surface: (1) Formation of a dative bond between the ether oxygen atom and a Si_{down} surface atom through donation into the empty p orbital; (2) nucleophilic attack of a nearby Si_{up} atom at C_α. The dots indicate unpaired electrons (dangling bonds). Copyright 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.



Results from bonding analysis (pEDA) provide proof for the proposed bonding models. (a) Donor-acceptor bonding in the DB structure shown by the charge flow from molecule to surface. (b)–(c) S_N2 type backside reaction from the neighboring silicon surface atom by moving charge in the LUMO (s*(C-O)-type orbital). Copyright 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.

Interfacial molecular packing determines exciton dynamics in molecular heterostructures: the case of pentacene – perfluoropentacene

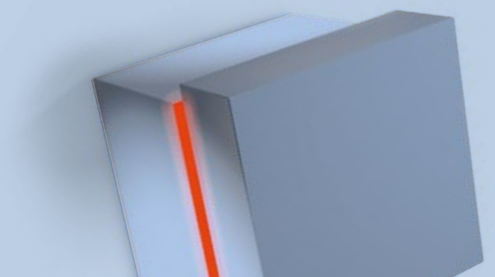
A. Rinn, T. Breuer, J. Wiegand, M. Beck, J. Hübner, R.C. Döring, M. Oestreich, W. Heimbrodt, G. Witte, S. Chatterjee

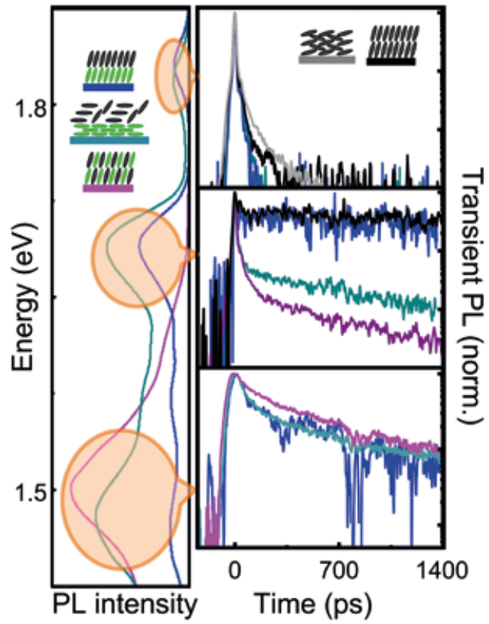
Applied Material Interfaces **9**, 42020 (2017)

Organic photovoltaics promise less materials use in low-cost offset-style printing of thin-film devices due to large absorption cross sections compared to conventional, e.g., silicon-based, photovoltaics. Furthermore, molecular materials may show enhanced efficiencies by singlet-exciton fission while large exciton binding energies may hinder efficient charge separation and, hence, current harvesting.

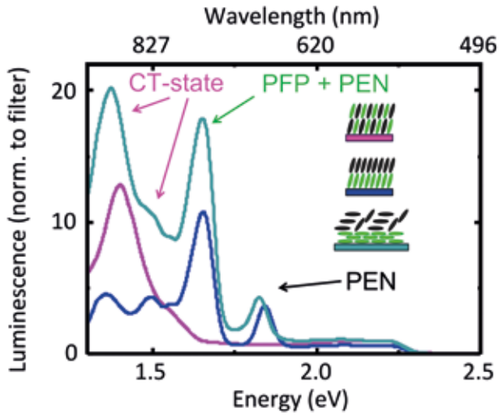
One of the key challenges in the field of organic photovoltaics is the separation of optically excited bound electron-hole pairs, so-called excitons. Of particular relevance are charge-transfer (CT) excitons at donor-acceptor interfaces with the electron in the acceptor and the hole in the donor molecule as they are prime candidates as intermediaries for charge separation. Studying these CT excitons in state-of-the-art devices is challenging as these consist of blends of molecular donors and acceptors in order to provide maximum internal interface area. The resulting complex interface geometry structure hampers microscopic characterization of such CT-excitons and, in particular, denies a well-defined correlation of the electronic properties with the molecular packing at the interface.

In combining their expertise in the fabrication of such highly ordered crystalline molecular heterostructures with precise, time-resolved optical microspectroscopy the groups from Marburg and Gießen successfully study the energetics and dynamics of CT-excitons at the donor-acceptor interface. The results show that the spatial separation of electrons and holes in the CT-excitons leads to extended lifetimes compared to the pristine species. Intriguingly, the energetics reveal that the common description of such excitons based on a straight-forward orbital picture as a mere linear combination of the involved individual constituents is insufficient and a more intricate description of CT-excitons is needed. These experimental data are the first to systematically investigate such excitations in highly-ordered crystalline molecular heterostructures which will enable further theoretical calculations on the involved electronic effects. Overall, the findings show that charge separation depends intricately on the molecular arrangement at the internal interface and hint that highly ordered organic photovoltaic devices could outperform disordered, nanocrystalline or even glassy structures.





Transient photoluminescence data for the indicated spectral regions on the prototypical donor-acceptor pair systems pentacene / perfluoropentacene. Reprinted with permission. Copyright 2017 American Chemical Society.



Characteristic spectrally resolved emission of the pristine materials and charge-transfer excitons for the various molecular stacking patterns illustrated in the inset. Reprinted with permission. Copyright 2017 American Chemical Society.

Lightwave valleytronics in a monolayer of tungsten diselenide

F. Langer, C.P. Schmid, S. Schlauderer, M. Gmitra, J. Fabian, P. Nagler, C. Schüller, T. Korn, P.G. Hawkins, J.T. Steiner, U. Huttner, S.W. Koch, M. Kira, R. Huber

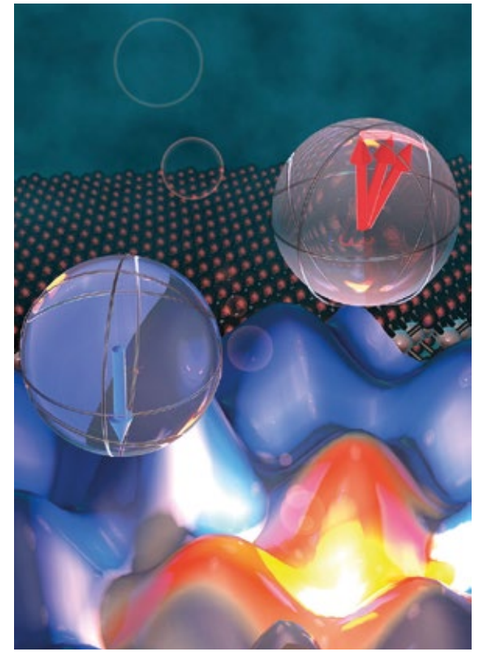
Nature **557**, 76 (2018)

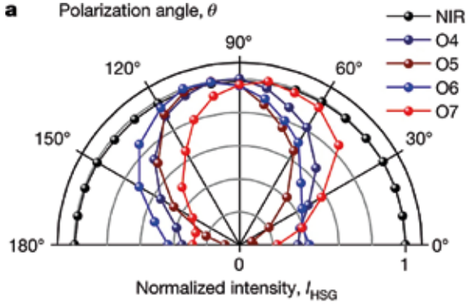
The next step in modern information technology, so-called quantum information technology, are robust and quickly switchable electronic states provided by "valley pseudospin" which can be changed when energized electrons are optically driven between distinct energetic valleys in hexagonal layered materials. Taking only a few femtoseconds to achieve and in room temperature air, "lightwave valleytronics" may take efficient storage, processing and communication beyond "Moore's law".

As a consequence of the hexagonal bandstructure in TMDCs, novel quantum aspects materialize as two different energy valleys appear at the K and K′ points of the Brillouin zone. Whether an electron resides in K or K′ valley or a superposition of both can be described by a spin-like quantity, the valley pseudospin. Electrons can be selectively excited in either of these valleys by using right- or left-circular polarized light. The aspiration to develop pseudospin-qubit operations (qubits can be mixtures, i.e. superpositions, of the 1 or 0 states) has prompted a novel research field dubbed “valleytronics”.

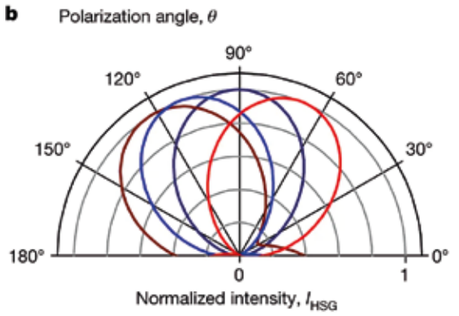
Using a combination of optimized optical and THz excitation pulses, the record-fast valley pseudospin switching is demonstrated in a monolayer of WSe_2. In the experiments, a strong terahertz light pulse accelerates the previously photo-generated charge carriers. As predicted by fully microscopic calculations, the flipping qubit was directly observed as changed circular polarization of light emitted by the electrons. More specifically, the experiment–theory team from Marburg, Regensburg and Michigan found that after excitation with circularly polarized light, the emission contained distinct opposite circular polarization due to the pseudo-spin flip. While the current experiment transfers 66% of valley-polarized electrons to the other valley, theory shows how a fidelity of 96% can be reached with slightly improved parameters, paving the way for developing room-temperature quantum signal processing.

Energy-landscape in a WSe_2-semiconductor depicted as blue hills. Electrons are accelerated from one valley to the next (yelloworange) with the colored arrows indicating change of the valley-pseudospin.





(a) Measured polarization-resolved intensity IHSG of individual side-band orders (normalized, colored data points) for circularly polarized excitation (normalized, black data points) of the K valley only. Reprinted by permission from Springer Nature Customer Service Centre GmbH. Copyright 2018.



(b) Computed polarization of high-order sidebands (orders four to seven, solid lines, same colors as in a) following a valley-selective excitation in the K valley. Reprinted by permission from Springer Nature Customer Service Centre GmbH.

Enhanced absorption by linewidth narrowing in optically excited type-II semiconductor heterostructures

M. Stein, C. Lammers, M.J. Drexler, C. Fuchs, W. Stolz, M. Koch

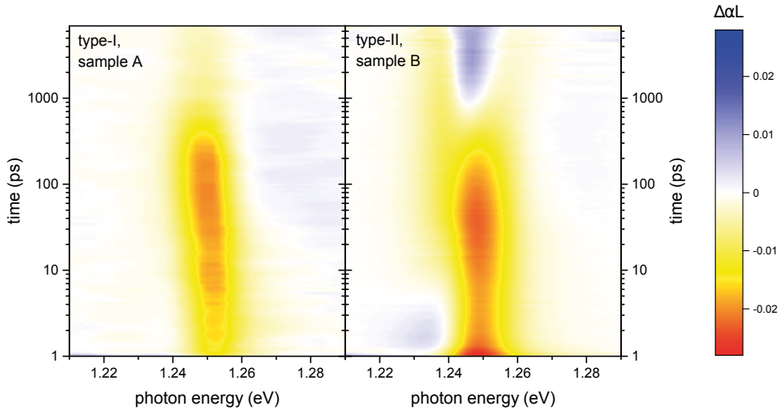
Physical Review Letters **121**, 017401 (2018)

Following optical excitation excitonic lines can show reduced absorption, shifts and broadening associated with optical nonlinearities arising from the many-particle nature of the system. Yet, experimental results for the first time show the opposite effect, i.e., a surprising linewidth narrowing of the direct exitonic 1s heavy-hole transition in a type-II quantum well system. The excitonic resonance in the linear absorption is spectrally sharper in the excited sample than in the unexcited sample.

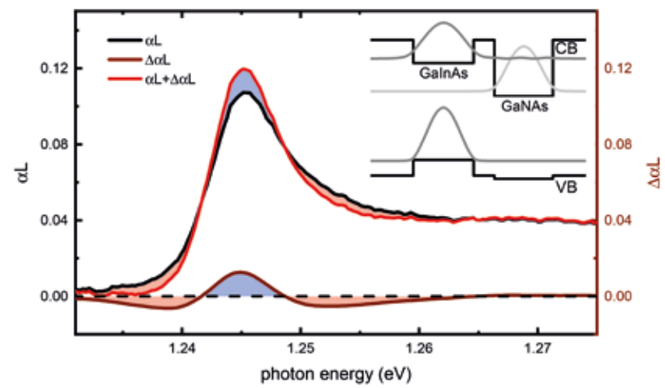
Quantum well (QW) based semiconductor heterostructures are ideal model systems to study the properties of low-dimensional carrier systems, explaining why the optical properties of these nanostructures have been extensively investigated over the last 30 years. At low temperatures excitonic resonances dominate the absorption spectrum. When optically excited these resonances typically broaden, shift and show a reduced absorption due to several many-particle effects including phase-space filling, band gap renormalisation, screening and excitation induced dephasing.

New experiments, however, reveal a surprising linewidth narrowing of the direct exitonic 1s heavy-hole (hh) transition in a type-II quantum well system. Type-II semiconductor heterostructures are characterized by two adjacent but different QWs, often with a barrier between them. The energy levels in the conduction and valence band are designed such that for a particular photon energy only one QW is excited and that subsequently either electrons or holes find energetically more favorable states in the other QW and undergo a spatial charge transfer.

The linewidth narrowing, which does not occur in a type-I reference sample, is observed in an optical pump-optical probe experiment with femtosecond pulses and builds up on a pico- to nanosecond timescale, with the actual speed depending on experimental parameters such as excitation density, temperature and barrier width. A direct attribution of this effect to known physical mechanisms did not become evident. This lays the case for further experimental and theoretical investigations on other charge-transfer systems, such as donor-acceptor systems or heterojunction solar cells, where the spatial charge transfer through an interface is essential for their operation.



Differential absorption spectra from a type-II sample (right) and from a reference sample with a type-I band alignment (left), illustrating the temporal behavior of the pump-induced changes of the optical absorption. Blue color shades indicate an excitation-induced increase of the linear absorption. Reprinted figure with permission. Copyright 2018 by the American Physical Society.



The linear absorption (black line) of a type-II heterostructure with a 6 nm thick GaAs intermediate barrier together with its differential absorption (dark red line) and the sum of linear and differential absorption (red line). The unexcited sample already shows a distinct 1 s excitonic resonance in the optical absorption at 1.245 eV. Nevertheless, an optical excitation can lead to an even sharper and more pronounced excitonic absorption (in type-II heterostructures). The differential absorption signature shown here occurs 5 ns after the optical excitation. The inset contains a schematic of the sample's band structure with the respective wave functions. Reprinted figure with permission. Copyright 2018 by the American Physical Society.

Subcycle observation of lightwave-driven Dirac currents in a topological surface band

J. Reimann, S. Schlauderer, C.P. Schmid, F. Langer, S. Baierl, K.A. Kokh, O.E. Tereshchenko, A. Kimura, C. Lange, J. Güdde, U. Höfer, R. Huber

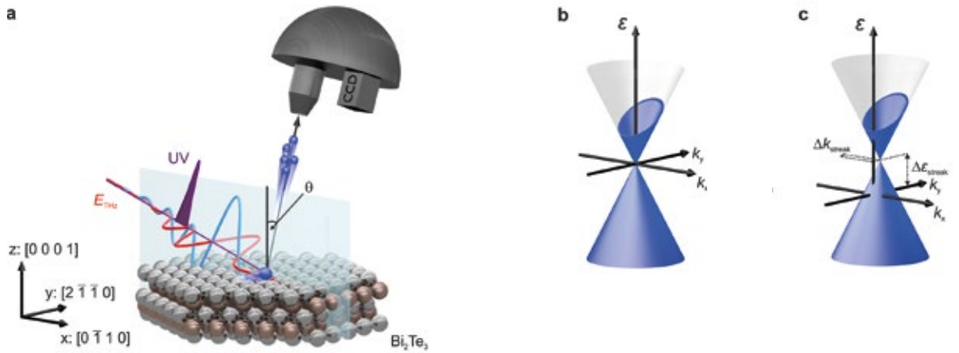
Nature **562**, 396 (2018)

The first subcycle angle-resolved photoemission study produced a band structure movie of electrical currents carried by Dirac electrons as they are driven by an intense THz wave. The investigated currents consist of spin-polarized electrons confined to the uppermost atomic layers of the topological insulator Bi_2Te_3. The electrons react in an inertia-free fashion to the driving field. Spin-momentum locking enables fully ballistic lightwave currents over several 100 nm.

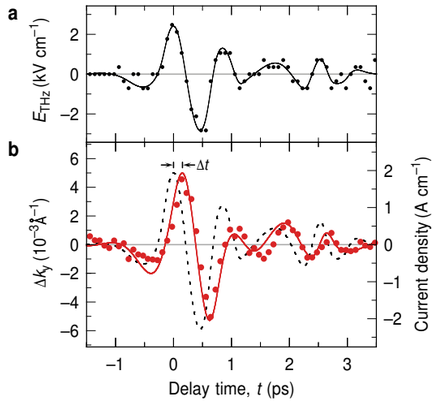
Lightwave electronics builds upon the idea that the electric field of intense light pulses can be used to accelerate electrons at terahertz to petahertz clock rates. Yet, in conventional semiconductors and dielectrics the finite band mass and ultrafast scattering limit the ballistic excursion and the velocity of the electrons. Reimann and collaborators have shown that the unique band structure of topological insulators lifts these constraints.

The work, a collaboration of SFB 1083 with researchers in Regensburg, Novosibirsk and Hiroshima, not only merges two novel and promising concepts in physics – topology and lightwave electronics. It also combines the expertise of the Huber group in Regensburg in manipulating electrons in solids with intense single-cycle terahertz (THz) transients, with the capabilities of time and angle-resolved photoelectron spectroscopy (ARPES) developed in Marburg. The experiment represents the first ARPES investigation with subcycle time resolution. It allows to observe how the carrier wave of a THz pulse accelerates Dirac fermions in the topological surface state (TSS) of Bi_2Te_3. While terahertz streaking of photo-emitted electrons traces the electromagnetic field at the surface, the acceleration of Dirac states leads to a strong redistribution of electrons in momentum space. This redistribution is mapped out directly in an ultrafast movie.

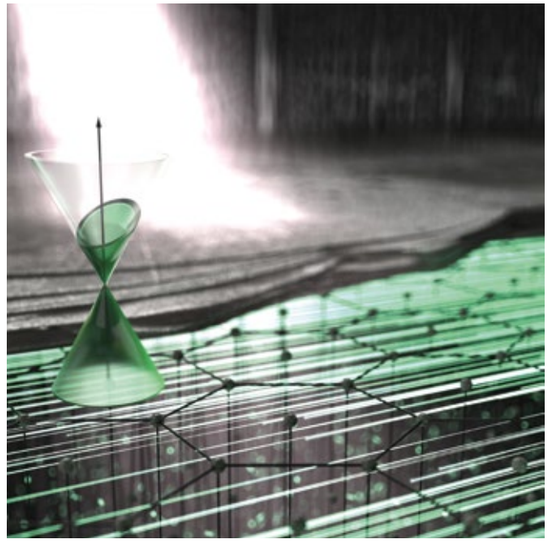
The experiments reveal that the electrons carrying the current react inertia-less on the accelerating field and travel with the Fermi velocity of 4.1 Å/fs or 410 nm/ps. The resulting surface currents reach peak densities as large as 2 Å/cm. Analysis with a semiclassical Boltzmann model shows that the relevant electron scattering times amount to at least 1 ps. These unique transport dynamics opens a realistic parameter space for lightwave electronics. Due to the large Fermi velocity, the low scattering rates, and the linear band structure, lightwave-driven Dirac fermions in TSSs may ballistically propagate in dispersion-free wavepackets over distances as large as several 100 nm. This distance easily exceeds the gate width of the latest electronic transistors by orders of magnitude. Owing to spin-momentum locking, the ballistic Dirac currents also carry a spin current, which could enable spintronics up to optical clock rates.



Concept of subcycle time- and angle-resolved photoemission spectroscopy. Reprinted by permission from Springer Nature Customer Service Centre GmbH. Copyright 2018.



Subcycle dynamics of electric current. Reprinted by permission from Springer Nature Customer Service Centre GmbH. Copyright 2018.



Artistic view of the experiment.

Lateral scattering potential of the PTCDA/Ag(111) interface state

A. Sabitova, R. Temirov, F.S. Tautz

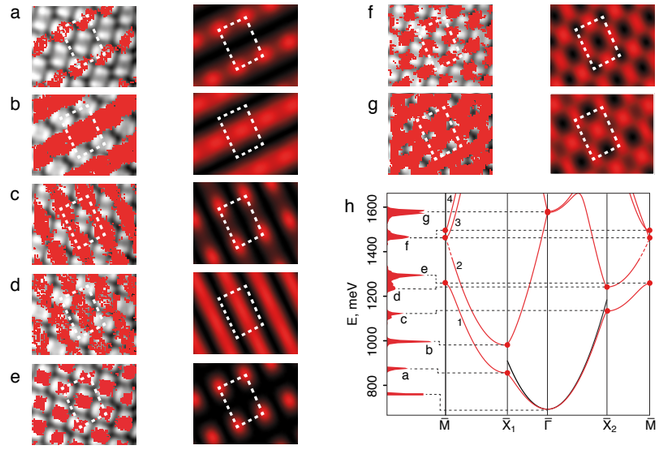
Physical Review B **98**, 205429 (2018)

Atomic-scale patterning of interfaces consisting of large organic molecules and metal surfaces allows the crafting of structures with novel electronic properties and, ultimately, designed quantum states. In this context, dispersive interface states are highly relevant as these are most susceptible to the effects of lateral structuring. To take full advantage of this approach to quantum state engineering, it is vital to first develop a detailed understanding of such molecule/metal interfaces in their native, unstructured form.

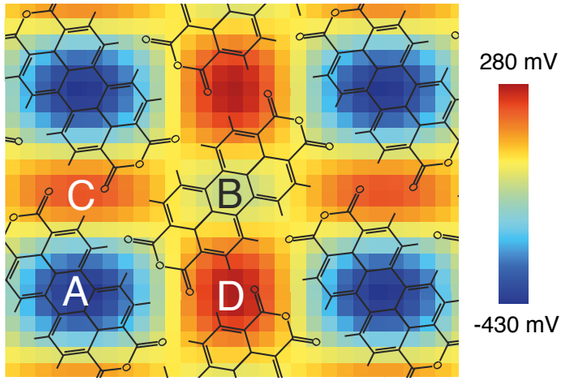
The interface of 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) with the Ag(111) surface was the first molecule-metal interface to reveal an unoccupied, parabolically dispersing two-dimensional (2D) interface state. Based on this finding, SFB-researchers have shown that an analytical one-dimensional (1D) model potential describes certain facets of the interface state very well. It is clear, however, that this 1D model cannot capture several other important aspects, most notably the scattering of electrons in the interface state by the molecular layer. This scattering is important since it could lead to the emergence of a true hybrid molecule-metal interface state.

Because the scattering is expected to impress its signature into the 2D band structure of the interface state, it is important to measure the latter. But although the PTCDA/Ag(111) interface is a well-studied prototype, its complete band structure had so far not been determined. Scanning tunneling spectroscopy (STS) is one of the few suitable techniques in the present case. However, STS has principal problems in providing band maps. These problems stem from the inevitable superposition of topographic and electronic image contrasts.

A newly developed technique of STS, called feature-detection STS, succeeds in eliminating the contribution of the surface topography, leaving behind a highly posterized image of the electronic structure. This allows a comprehensive determination of the band structure of the PTCDA/Ag(111) interface state. Evidence suggests a very strong scattering of the surface state electrons by the molecular layer. Surprisingly, this scattering is attractive, which supports the idea of an emergent hybrid interface state, and limited to only one of the two sublattices. The latter observation could be the key to understanding certain observations regarding the lifetime of interface state electrons.



Band structure of the PTCDA/Ag(111) interface state as derived from feature-detection STS and a fitted nearly-free electron model calculation. Reprinted figure with permission. Copyright 2018 by the American Physical Society.



Scattering potential of the PTCDA/Ag(111) interface state as derived from feature-detection STS and a fitted nearly-free model calculation. Reprinted figure with permission. Copyright 2018 by the American Physical Society.

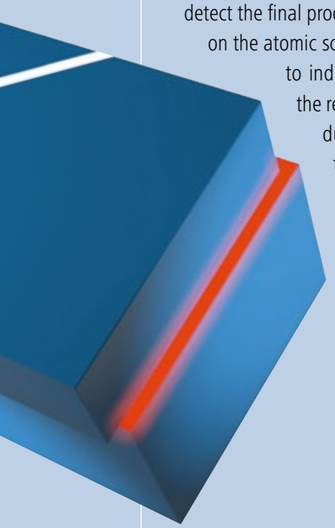
Controlling an S_N2 reaction by electronic and vibrational excitation – tip-induced ether cleavage on Si(001)

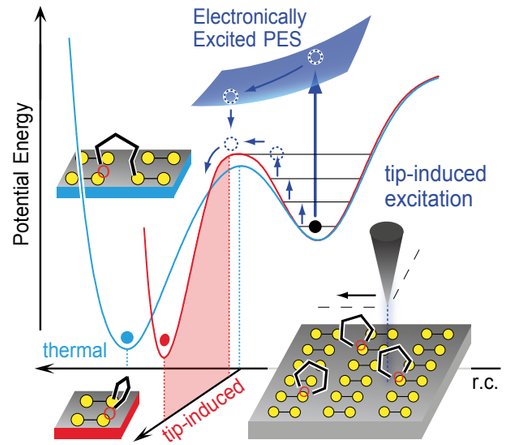
G. Mette, A. Adamkiewicz, M. Reutzel, U. Koert, M. Dürr, U. Höfer

Angewandte Chemie – International Edition **58**, 3417 (2019)

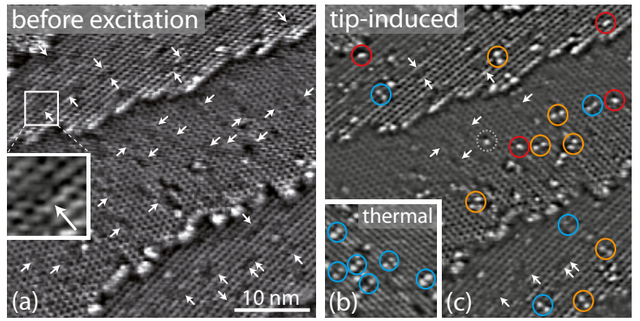
New ways for controlling organic reactions on silicon surfaces – better control of surface reactions, in particular of organic molecules on inorganic surfaces, will ultimately lead to the formation of better interfaces between inorganic substrates and organic multilayers grown on these substrates. In a joint effort, the groups from Gießen and Marburg used scanning tunneling microscopy for controlling the final products of a textbook-type reaction of organic molecules on silicon surfaces.

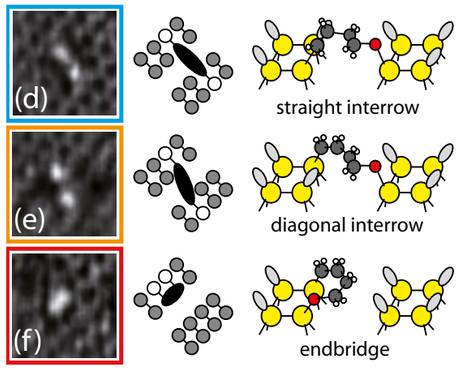
Ether cleavage on silicon is the surface analogue of an S_N2 reaction; S_N2 reactions represent the textbook example for how to control solution-based chemical reactions by means of steric hinderance or the choice of solvent. The team around Gerson Mette and Michael Dürr has shown a new possibility for controlling this type of reaction. Using a scanning tunneling microscope (STM), they could not only detect the final products of such a reaction with resolution on the atomic scale but made use of the tip of the STM to induce the reaction itself. When imaging the reaction products, they found that tip-induced ether cleavage on Si(001) leads to additional final products which are not obtained by thermal activation, the latter being the "classical" way of activating the reaction. Moreover, different final products can be selectively realized by different excitation channels, either direct excitation by electron transfer or multiple excitation of vibrational modes induced by the tunneling electrons. As the two channels can be selectively addressed by the tunneling bias, a new way of controlling the reaction and its final products is achieved. In more general, the results show the potential for controlling chemical reactions on surfaces through different excitation mechanisms. The results are also applicable to a wide range of on-surface reactions of organic molecules and open control of these reactions beyond the limitations of thermally activated reaction schemes.





Tip-induced ether cleavage leads to new final products when compared to thermal excitation. The different final products can be selectively addressed by the type of excitation. Copyright 2019 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.





STM images before (a) and after (c) tip-induced ether cleavage. Additional configurations are observed when compared to thermal activation (b). (d) to (f) blow ups and schematic representations of the observed configurations. Copyright 2019 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.

Molecular topology and the surface chemical bond: alternant versus nonalternant aromatic systems as functional structural elements

B.P. Klein, N.J. van der Heijden, S.R. Kachel, M. Franke, C.K. Krug, K.K. Greulich, L. Ruppenthal, P. Müller, P. Rosenow, S. Parhizkar, F.C. Bocquet, M. Schmid, W. Hieringer, R.J. Maurer, R. Tonner, C. Kumpf, I. Swart, J.M. Gottfried

Physical Review X **9**, 011030 (2019)

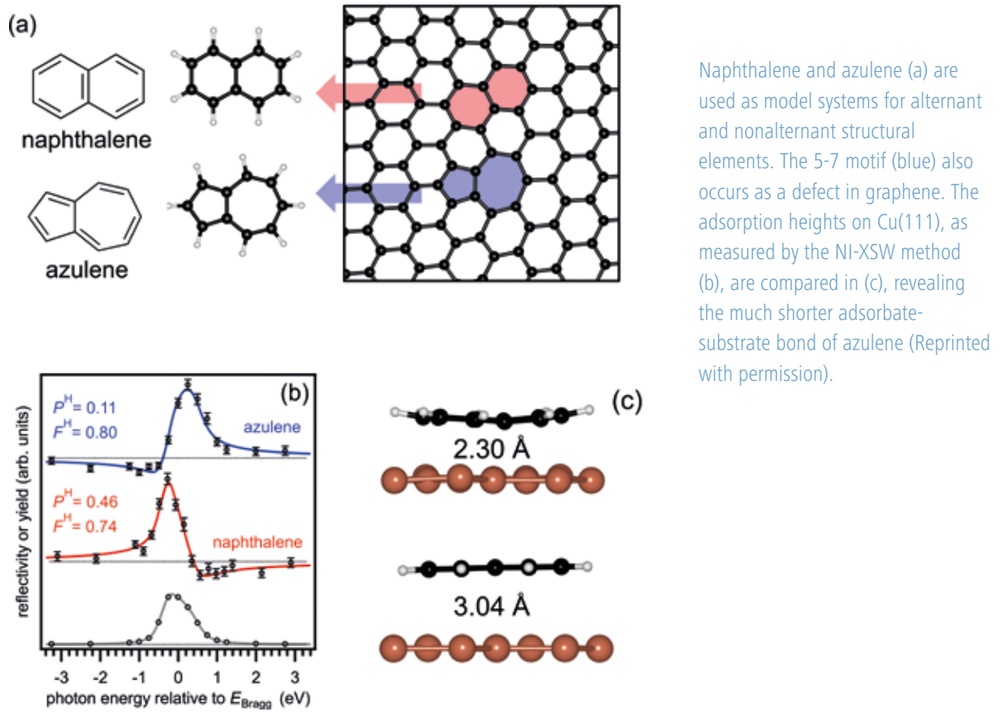
How an organic semiconductor bonds to a metal surface depends on the linking pattern of its carbon atoms. By comparing the aromatic, structurally isomeric, molecules naphthalene and azulene, it was shown that the unusual 5-7 ring system of azulene bonds much stronger to a metal surface than the 6-6 ring system of naphthalene. The knowledge gained from this model system is valuable in tuning the properties of metal-organic interfaces in organic electronic devices. It also sheds new light on how metals interact with graphene, in which azulene-like structural elements occur as defects.

In so-called organic electronic devices, such as modern displays with organic light-emitting diodes (OLEDs), organic materials connect to metal contacts. The resulting metal–organic interfaces determine important performance parameters such as rates of charge-carrier injection. Precise control over the interface properties, especially the wave-function overlap and the energy-level alignment, is therefore critical for developing improved devices. Here, several SFB 1083 projects together with international collaborators showed that the properties of metal-organic interfaces depend strongly on the topology, i.e., the linking pattern of the atoms in the π-electron system, of the organic molecule.

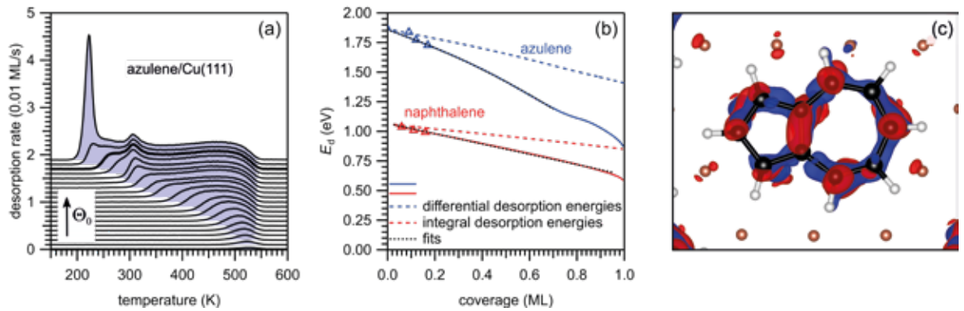
Organic semiconductors are typically based on adjoined hexagonal rings, like in graphene. This linking pattern is described as an alternant topology. Nonalternant topologies, which occur when the structure contains, for example, five- or seven-sided rings, have rarely been considered. To elucidate the influence of the topology on the interaction with a copper surface, the aromatic hydrocarbon naphthalene, which has an alternant topology, is compared with its nonalternant isomer, azulene.

This study reveals that azulene forms a much stronger and shorter bond to a copper surface than naphthalene. Spectroscopic analysis of the electronic structure shows that azulene forms a true chemical bond and receives negative charge from the surface, whereas naphthalene bonds only weakly and does not exchange charge. Theoretical analysis finds that the influence of the topology on the electronic structure, especially the lowest unoccupied molecular orbital (LUMO), is responsible for the different behavior.

Based on these findings, it is proposed that nonalternant structural elements can be used to optimize performance-related properties of functional metal-organic interfaces. In addition, graphene defects with nonalternant topology, such as Stone-Wales defects, are expected to interact more strongly with metals than regular graphene, which is important for the electric contacting of carbon-based 2D materials in electronic devices.



Naphthalene and azulene (a) are used as model systems for alternant and nonalternant structural elements. The 5-7 motif (blue) also occurs as a defect in graphene. The adsorption heights on Cu(111), as measured by the NI-XSW method (b), are compared in (c), revealing the much shorter adsorbate-substrate bond of azulene (Reprinted with permission).



Analysis of the temperature-programmed desorption data in (a) confirms that azulene has a higher adsorbate-substrate interaction energy (b) over the whole monolayer coverage range. The bond of azulene to Cu(111) is associated with massive electron transfer from the surface to the LUMO of the molecule, as is illustrated in (c) (Reprinted with permission).

A solvent-free solution: Vacuum-deposited organic monolayers modify work functions of noble metal electrodes

F. Widdascheck, A.A. Hauke, G. Witte

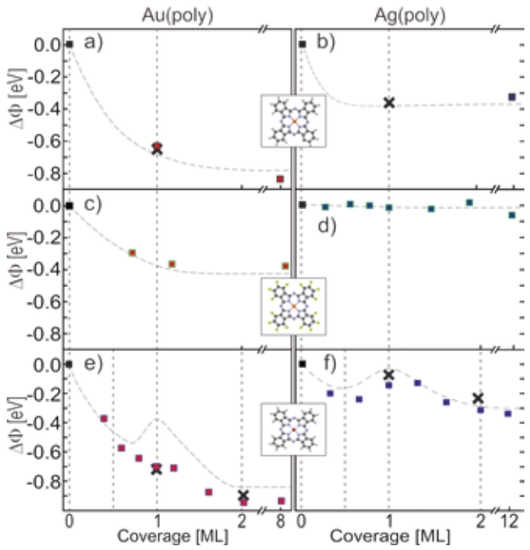
Advanced Functional Materials **29**, 180385 (2019)

Work function tailoring by organic monolayers is one of several promising approaches to reducing contact resistance between metal electrodes and organic semiconductors in organic electronics devices. In this study, several polar and non-polar phthalocyanines were used to modify the work functions of noble metal electrodes, for both single-crystalline model surfaces and actual polycrystalline electrodes.

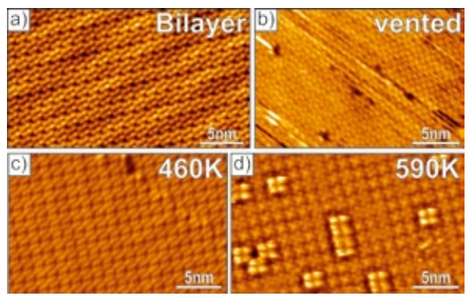
Atomically flat, ultra-pure single-crystal surfaces allow detailed scanning tunneling microscopy (STM) studies of the adsorption geometry of organic molecules on noble metals. Combining this with an in-situ Kelvin probe setup allows investigation of the change in work function of noble metals as a function of coverage of molecular adsorbates. For the case of phthalocyanines on Au(111) surfaces, a general reduction in work function with increasing molecular coverage can be observed within the first two monolayers due to the formation of interface dipoles between the metal and the phthalocyanine's carbon backbone. Beyond this coverage, the effect saturates.

The exact extent of this reduction depends on the properties of the chosen molecule: Fluorination for example weakens the effect (observed here for F_{16}CuPc), while the presence of an inherent molecular dipole (e.g. TiOPc) strengthens it. In addition, presence of TiOPc also leads to the formation of a local maximum around the completion of the first monolayer, which is due to the interplay between interface dipoles and molecular dipoles. Similar observations can be made for Ag(111), where the overall reduction is, however, far less pronounced and in the case of F_{16}CuPc not evident at all.

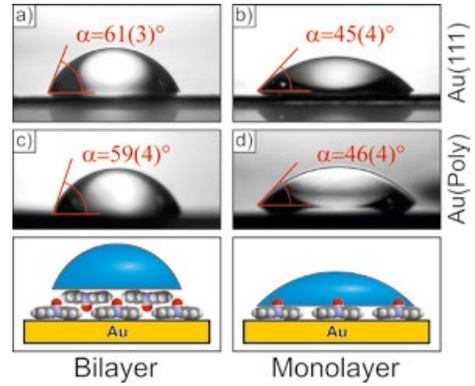
Kelvin probe analysis on the type of polycrystalline Au and Ag surfaces relevant for device applications reveals an analogous behavior. Here, higher surface roughness and energetic disorder leads to an altogether reduced effect. For both poly- and single-crystalline metal surfaces, it further appears to be possible to form well-defined monolayers of non-fluorinated phthalocyanines simply by thermal desorption of previously deposited multilayers, such that only the more strongly bound monolayer remains on the substrate. The work functions of thus-produced contact primers match those of the as-deposited monolayers in all cases. For polar phthalocyanines, it is even possible to produce a well-defined bilayer due to interaction of the permanent molecular dipoles. These dipoles further allow differentiation between monolayer- and bi-/multilayer coverage by simple water contact angle measurements. Lastly, this method allows exposure of the phthalocyanine multilayers to the air, then form well-ordered monolayers in vacuum by thermal desorption which exhibit the same properties as contact primers not exposed to air.



Metal work function changes upon adsorption of a, b) CuPc , c, d) F_{16}CuPc and e, f) TiOPc. Square data points show incremental deposition, crosses refer to multilayer desorption. Dashed grey lines indicate the results for the (111) surfaces. Copyright 2019 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.



140×140 nm² STM micrographs of TiOPc bi-(a-c) and monolayer (d) films on Au(111), prepared by multilayer desorption. Copyright 2019 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.



Water contact angle in ambient conditions: a) and c) TiOPc bilayer prepared by multilayer desorption, b) and d) TiOPc monolayer prepared by multilayer desorption. Copyright 2019 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Quantitative imaging of electric surface potentials with single-atom sensitivity

C. Wagner, M.F.B. Green, M. Maiworm, P. Leinen, T. Esat, N. Ferri, N. Friedrich, R. Findeisen, A. Tkatchenko, R. Temirov, F.S. Tautz

Nature Materials **18**, 853 (2019)

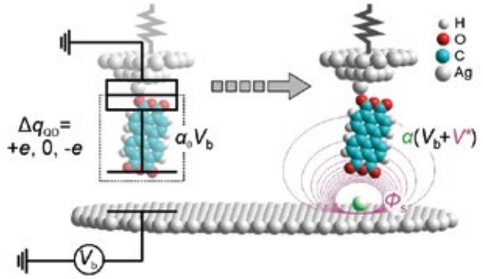
Coulomb interaction's long range allows large-scale structures and their electric signals to outshine smaller ones. This makes isolation and quantification of electric potentials originating from nanoscale objects (atoms or molecules) very challenging. A newly developed non-contact scanning probe technique employs a quantum dot sensor and joint electrostatic screening by tip and surface, thus enabling quantitative surface potential imaging across all relevant length scales down to single atoms.

Electrostatic interaction is key to the functionality of many nanoscale materials and systems including the performance of organic and inorganic semiconductor devices which are affected by electric dipoles at the relevant interfaces. As the few-nanometer scale becomes evermore relevant in device concepts, the ability to measure microscopic electric potentials in functional materials and devices becomes an increasing necessity. It is these electric potentials that can provide valuable insight into primary mechanisms at surfaces and interfaces, such as reconstruction or relaxation, mechanical distortion, charge transfer and chemical interaction, which all create electric potentials at the atomic scale.

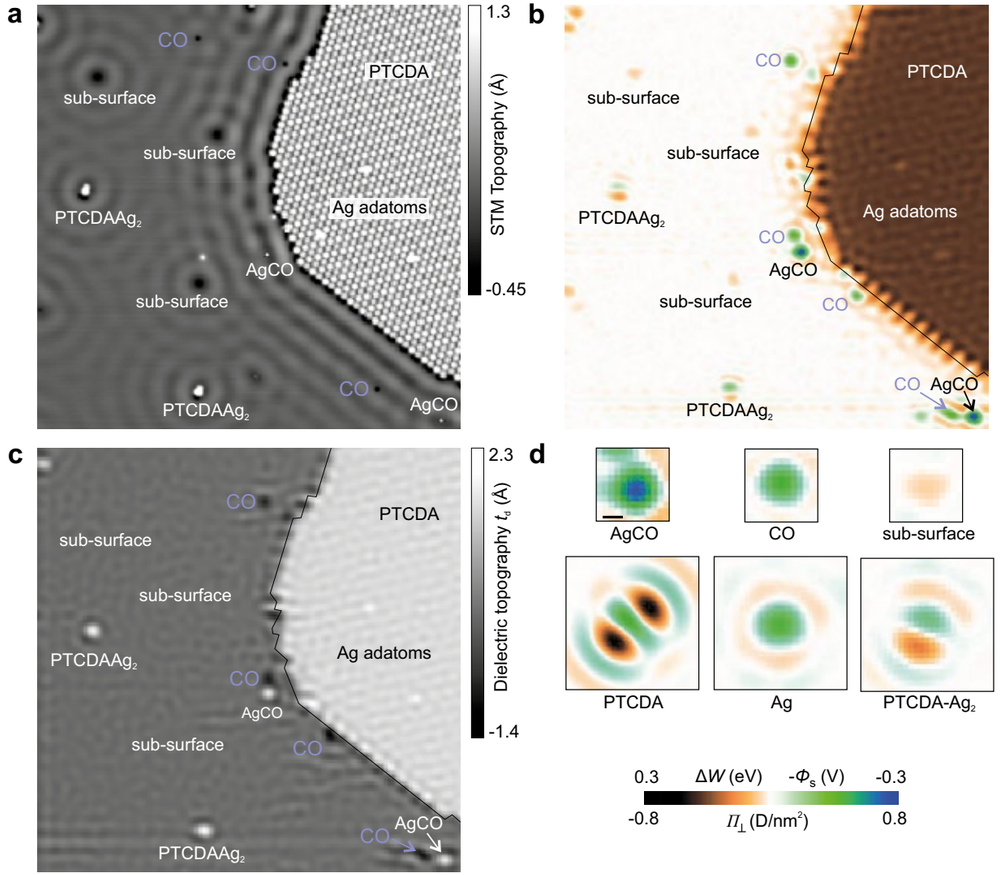
State of the art in electric potential imaging at surfaces is Kelvin probe force microscopy (KPFM), but at the level of single atoms or molecules and novel semiconductor devices, KPFM is problematic as high resolution imaging can only be reached at small tip–surface distances, i.e., where chemical forces start acting and interfering with a quantitative interpretation of the data.

A novel technique called scanning quantum dot microscopy (SQDM) may solve this problem. In this approach a single molecule is attached to the tip of a non-contact atomic force/scanning tunnelling microscope (NC-AFM/STM) by controlled manipulation. The molecule may then act as a quantum dot (QD) and can be used as a sensor to detect and image electric potentials. Rigorous analysis of the corresponding imaging mechanism, by making use of the formalism of electrostatic boundary value problems, shows that SQDM can indeed be used to quantitatively map out surface potential distributions and dielectric surface topographies.

In addition, the observed effect of the screening action of the combined tip/surface system inducing an exponential decay of electric potentials with lateral distance from the probing tip allows for an exceptionally high lateral resolution of the SQDM. Detailed investigation of this exponential screening forms the basis of an image deconvolution algorithm that, together with far-reaching instrumental developments, transforms SQDM into a powerful imaging technique for electric surface potential imaging in ever smaller nanostructures and novel materials.



Principle of electric potential sensing with a molecular quantum dot. Reprinted by permission from Springer Nature Customer Service Centre GmbH. Copyright 2019.



SQDM images of nanostructures on Ag(111). (a) STM image (60 × 60 nm^2) showing various adsorbates and defects on a Ag(111) surface. (b) SQDM surface potential image. (c) SQDM dielectric topography image. (d) SQDM images of individual nanostructures including a PTCDA–Ag_2 complex. Scale bar, 1 nm. Reprinted by permission from Springer Nature Customer Service Centre GmbH. Copyright 2019.

$[\{(PhSn)_3SnS_6\}\{(MCp)_3S_4\}]$ (M = W, Mo): minimal molecular models of the covalent attachment of metal chalcogenide clusters on doped transition metal dichalcogenide layers

E. Dornsiepen, F. Pieck, R. Tonner, S. Dehnen

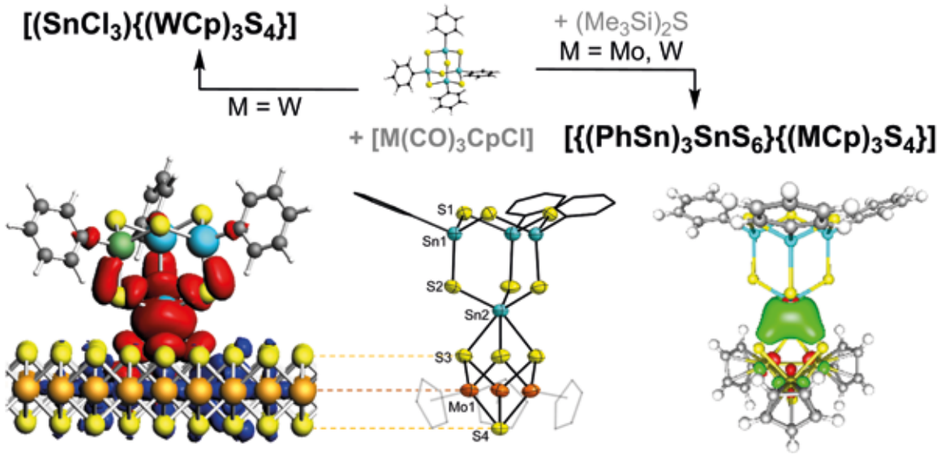
Journal of the American Chemical Society **141**, 16494 (2019)

Transition metal dichalcogenides (TMDCs) with their 2D-structure promise huge potential in electronic applications which drives the search for novel TMDC-heterostructures. Synthesis of molecular model systems for the up to now unknown adsorption of organotin chalcogenide cluster molecules on TMDC surfaces is an important step. Computational studies reveal similar covalent bonding interactions for the model system as well as for the adsorption on a TMDC surface.

TMDC heterostructures with other 2D materials have already proven useful in tunneling transistors or solar cells. Hybrid systems with layers of adsorbed molecules show optoelectronic application potential, as they allow tailoring of electronic properties and high photoabsorption of molecular materials. Here, organic molecules like pentacene or coordination compounds like phthalocyanines interact with the TMDC surface by means of dispersion interactions. The interaction of larger organometallic systems with TMDCs, however, has not yet been studied, partially due to the fact that the chemisorption of molecules on TMDC surfaces is relatively weak, hence adsorbents tend to randomly move around.

With the aim to mimic the yet unknown covalent deposition of metal chalcogenide clusters on MoS_2 or WS_2 layers, and thereby explore the interaction between the two systems and potential consequences for the physical properties, the authors synthesized heterobimetallic model systems. $[(SnCl_3)(WCp)_3S_4]$, $[\{(PhSn)_3SnS_6\}\{(MoCp)_3S_4\}]$, and $[(PhSn)_3SnS_6\{(WCp)_3S_4\}]$ were obtained in ligand exchange reactions from $[(PhSn)_4S_6]$ and $[M(CO)_3CpCl]$ (M = Mo, W). Indeed, the $\{M_3S_4\}$ cages in the three compounds resemble a section of the respective TMDC monolayers, altogether representing minimal molecular model systems for the adsorption of organotin sulfide clusters on MoS_2 or WS_2. The interaction between the $\{(MCp)_3S_4\}$ and $\{(PhSn)_3SnS_6\}$ subunits is characterized by multicenter bonding, rendering the respective Sn atom as Sn(II), hence driving the clusters into a mixed-valence Sn(IV)/Sn(II) situation, and the M atoms as M(IV) upon an in situ redox process. The attachment is thus weaker than via regular covalent M–S bonds, but definitely stronger than via van der Waals interactions that have been characteristic for all known interactions of molecules on TMDC surfaces so far.

Calculations of a periodic model system that simulates the attachment of the $\{(PhSn)_3S_6\}$ fragment to MS_2 surfaces reveal striking similarities in structure and bonding situation, given the MS_2 surfaces are doped with titanium or other electron-poor metal atoms. This renders the new compounds as relevant molecular models for covalent attachment of larger organometallic systems on TMDCs.



$[(SnCl_3)(WCp)_3S_4]$ (1), $[\{(PhSn)_3SnS_6\}\{(MoCp)_3S_4\}]$ (2), and $[(PhSn)_3SnS_6\{(WCp)_3S_4\}]$ (3) are minimal molecular models of the yet unknown covalent deposition of metal chalcogenide clusters on transition metal dichalcogenide (TMDC) layers, as shown by a combined experimental and theoretical work. Reprinted with permission. Copyright 2019 American Chemical Society.

Template-controlled on-surface synthesis of a lanthanide supernaphthalocyanine and its open-chain polycyanine counterpart

Q. Fan, J.-N. Luy, M. Liebold, K. Greulich, M. Zugermeier, J. Sundermeyer, R. Tonner, J.M. Gottfried

Nature Communications **10**, 5049 (2019)

Phthalocyanines possess unique optical and electronic properties and thus are widely used in (opto)electronic devices, coatings, photodynamic therapy, etc.. Extending the π-conjugation of phthalocyanine dyes, while synthetically challenging, has the potential to produce desirable new molecular materials.

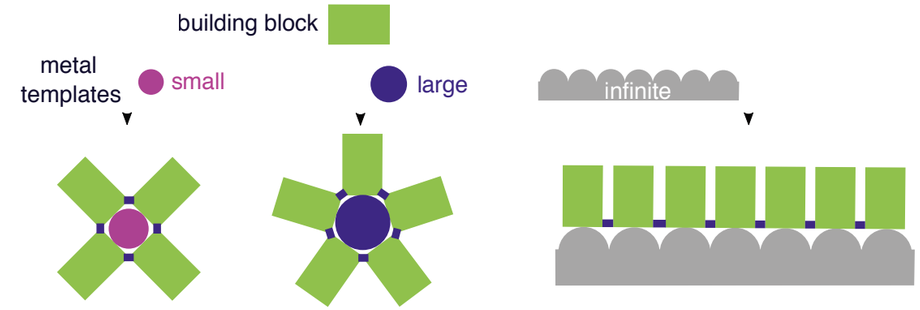
On-surface synthesis is a versatile complement to chemical synthesis in solution. The reactions are typically performed on solid surfaces under clean vacuum conditions. This approach is especially advantageous for reactants and products of low solubility. Hence, on-surface synthesis is applied to obtain low-dimensional materials, such as 1D polymers and 2D covalent organic frameworks.

Surfaces influence reactions in multiple ways by affecting the rates at which bonds are formed and broken, by favoring certain reaction outcomes or, e.g., confining the reaction to two dimensions. This knowledge provides an additional means to control the outcome of a reaction: choosing a surface with the right composition and structure can steer the reaction in a way that the desired product is obtained.

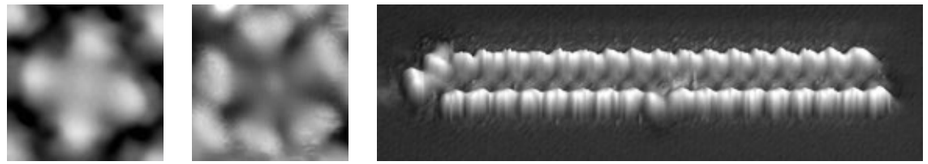
The authors previously used the popular surface Ullmann reaction to make shape-persistent macrocycles including honeycombenes and cycloarenes with different sizes and topologies. As the formation of macrocycles (rings) persistently competes with the formation of polymer chains, Qitang Fan and his colleagues developed a novel coordination template synthesis on surfaces to guide the formation of macrocycles. This synthesis is not based on the Ullmann reaction, but works with nitrile groups.

It is well-known in surface coordination chemistry that metal atoms with different sizes may coordinate different numbers of functional nitrile groups by acting simultaneously as catalyst and template. In their template the authors for the first time chose lanthanide metal atoms, which in solution chemistry react with dicarbonitriles to form bulky bis(phthalocyaninato) double-decker complexes.

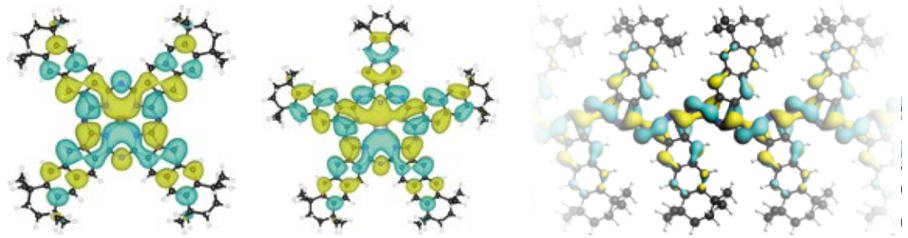
Based on their ideas, the authors selected a naphthalenedicarbonitrile precursor on a silver (111) surface. With gadolinium (Gd) as the template metal, a superphthalocyanine formed, the first of its kind without uranium as the metal center. In a next step, the silver surface itself was used as a virtually infinite template. In this way, polycyanine chains, which can be considered the open-chain counterparts of the cyclic phthalocyanine and superphthalocyanine complexes, developed. These polycyanine chains provide an intriguing model for an organic semiconducting polymer with an absorption band in the visible range.



The strategy: coordination template synthesis on a metal surface (Reprinted with permission).



Scanning tunneling microscopic images of the reaction product topology. (Reprinted with permission)



Orbitals: Lowest unoccupied molecular orbitals of Fe-NPc and Gd-SNPc, lowest unoccupied crystal orbital of polycyanine, from density-functional theory calculation (Reprinted with permission).

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Angewandte Chemie – International Edition **52**, 11202 (2013).

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Doctoral Dissertations

2014

1 Carolin R. Braatz (Physics, Marburg, 04/2014)
Wachstum, thermische Entwicklung und Phasentransformationen von NTCDA und Tetracen auf der Ag(111)-Oberfläche

2 Kristina Brixius (Physics, Marburg, 05/2014)
Nichtlineare optische Spektroskopie an der Galliumphosphid-Silizium(001)-Grenzfläche

3 Benjamin Breddermann (Physics, Marburg, 07/2014)
Effektive Behandlung der Coulomb-Streueffekte in der Vielteilchentheorie optisch angeregter Halbleiter

4 Kolja Kolata (Physics, Marburg, 09/2014)
Exciton dynamics in perfluoropentacene single crystals

5 Zhiliang You (Chemistry, Marburg, 12/2014)
Investigations of ferrocenyl-functionalized organotin chalcogenide and oxide complexes

6 Christoph Heyl (Physics, Marburg and Lund, 12/2014)
Scaling and gating attosecond pulse generation

2015

7 Marcus A. Lipponer (Physics, Marburg, 02/2015)
Untersuchungen zur Adsorptionsdynamik von Tetrahydrofuran, Trimethylamin und Cyclooctin auf Silizium-(001)

8 Ahmed B.M. Ibrahim (Chemistry, Marburg, 05/2015)
Axially and peripherally substituted phthalocyanine and azaphthalocyanine complexes for heterojunction design

9 Eliza Leusmann (Chemistry, Marburg, 06/2015)
Untersuchungen zur Anbindung von organischen Liganden an Sn/S-Cluster zum potenziellen Einfang von Übergangsmetall-Ionen

10 Marc Raupach (Chemistry, Marburg, 06/2015)
Quantenchemische Untersuchungen zur chemischen Bindung an Oberflächen, Entwicklung und Anwendung einer Energie-Dekompositions Methode

11 Niels Münster (Chemistry, Marburg, 09/2015)
Beiträge zur Chemie funktionalisierter ś-Bromsulfone, Cyclooctine und Diazaacene

12 Jonas Schwaben (Chemistry, Marburg, 11/2015)
Synthese des Molekülgerüsts von Synoxazolidinon A und Synthese und Molekulare Eigenschaften neuer 6,13-disubstituierter Pentacene

13 Michael Drexler (Physics, Marburg, 12/2015)
Zur Dynamik bestimmter Ladungsträger-Transferprozesse in Halbleiterquantenfilmen

14 Norman Born (Physics, Marburg, 12/2015)
Filterkonzepte für den Terahertz-Frequenzbereich

2016

15 Min Chen (Chemistry, Marburg, 03/2016)
Surface-assisted chemistry at interfaces between metals and organic thin films

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Nanojoule adsorption calorimetry: design, construction, novel evaluation approach, software development, characterization, and exemplary measurements

17 Martin Liebold (Chemistry, Marburg, 07/2016)
Synthesis and photophysical characterization of new azaphthalocyanines and azanaphthalocyanines for semiconductor interface design

18 Christian Berger (Physics, Marburg, 07/2016)
Microscopic theory of semiconductor laser material systems

19 Alexander Mänz (Physics, Marburg, 12/2016)
Über den Einfluss von Phthalocyanin-Monolagen auf die Struktur organischer Dünnfilme auf Metalloberflächen

20 Ulrich Huttner (Physics, Marburg, 12/2016)
Theoretical analysis of strong THz-field effects in semiconductors

21 Christoph Möller (Physics, Marburg, 12/2016)
Realization and experimental analysis of W-type III/V laser

2017

22 Michael Klues (Physics, Marburg, 02/2017)
Modellsysteme organischer Halbleiter: Präparation, Charakterisierung und Interpretation

23 Frederic Wagner (Chemistry, Marburg, 04/2017)
Studien zur Synthese eines substituierten Pentacens

24 Andreas Namgalies (Physics, Marburg, 07/2017)
Energietransfer angeregter Zustände in dünnen Schichten PTCDA auf Ag(111) und Au(111)

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Electron microscopy characterization of pentacene and perfluoropentacene grown on different substrates

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Untersuchungen zur Synthese und Reaktivität von Organozinnselenidclustern

27 Lisa Pecher (Chemistry, Marburg, 10/2017)
Adsorption dynamics and bonding analysis of organic molecules on silicon(001) surfaces

28 André Rinn (Physics, Marburg, 10/2017)
Correlating structural and optical properties in aromatic semiconductor crystals and heterostructures

29 Han Han (Physics, Marburg, 11/2017)
Quantitative evaluation of the interfaces in III/V semiconductors with scanning transmission electron microscopy

30 Lukas Nattermann (Physics, Marburg, 11/2017)
MOVPE growth studies on dilute bismide containing III/Vs & development of an MOVPE in-situ gas phase analysis setup

31 Sebastian Gies (Physics, Marburg, 12/2017)
Optical spectroscopy of functionalized semiconductor heterostructures: investigation of III-N-V/Silicon and III-Sb-V/GaAs heterostructures for laser applications

32 Christian Fuchs (Physics, Marburg, 12/2017)
Epitaxial growth and characterization of GaAs-based type-II (GaIn)As/Ga(AsSb)/(GaIn)As "W"-quantum well heterostructures and lasers

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Über die Dynamik des Charge-Transfer-Exzitons

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Vibrational and structural properties of ultrathin hetero-organic films

35 Janina Keller, née Felter (Physics, Jülich, 05/2018)
Different growth modes of molecular adsorbate systems and 2D materials investigated by low-energy electron microscopy

36 Alexander Lerch (Physics, Marburg, 06/2018)
Über unbesetzte elektronische Zustände und die Dynamik des Ladungstransfers an der TiOPc/Ag(111)-Grenzfläche und an PTCDA/TiOPc-Heteroschichten

37 Malte Zugermeier (Chemistry, Marburg, 08/2018)
Reactive aromatic molecules on metal surfaces: syntheses, reactions and structures

38 Robin Döring (Chemistry, Marburg, 08/2018)
Semiconductor-metal interfaces – comparison of planar and molecular systems using ultrafast pump-probe techniques

39 Christian Länger (Chemistry, Gießen, 08/2018)
Untersuchung der Adsorption organischer Moleküle auf Si(001) sowie ioneninduzierter Desorptionsphänomene auf H/Si(001) mittels XPS und STM

40 Han Zhou (Chemistry, Marburg, 09/2018)
Reactive metal-organic interfaces studied with adsorption calorimetry and photoelectron spectroscopy

41 Eduard Baal (Chemistry, Marburg, 09/2018)
1,2-Diazadibenzoperylene und 1,9-Dimethyldibenzoperylene: Über reduktive Aromatisierung zu vierfach funktionalisierten Polyaromaten

42 Jan Kuhnert (Physics, Marburg, 10/2018)
Optische und magneto-optische Untersuchungen an zweidimensionalen Übergangsmetalldichalkogeniden und deren Heterostrukturen

43 Johannes Reimann (Physics, Marburg, 11/2018)
Ladungsträgerdynamik und Photoströme im Dirac-Kegel topologischer Isolatoren

44 Malcolm Bartlett (Chemistry, Marburg, 12/2018)
Synthesis and photophysical investigation of axially and peripherally modified phthalocyanines for improved light-harvesting and photoreactivity

2019

45 Michel Blitz, née Fischer (Chemistry, Marburg, 03/2019)
Synthesis of substituted cyclooctynes and chemo-selectivity studies on multilayers using acetylene-cycloalkynes and bis azides using UHV-CVD

46 Paul Nikodemiak (Chemistry, Marburg, 03/2019)
Synthese von 1,2,4-Oxadiazolen, Cyclooctinen und Studien zur Synthese nicht-symmetrischer partiell fluorierter DNTT

47 Markus Stein (Physics, Marburg, 07/2019)
Dynamics of excitons in semiconductors

48 Eike Dornsiepen (Chemistry, Marburg, 07/2019)
Organotetrelchalkogenidcluster mit Heteroadamantanstruktur

49 Pirmin Kükelhan (Physics, Marburg, 08/2019)
Quantitative scanning transmission electron microscopy for III-V semiconductor heterostructures utilizing multi-slice image simulations

50 Jürgen Belz (Physics, Marburg, 10/2019)
Analysis of strain relaxation, ion beam damage and instrument imperfections for quantitative STEM characterization

51 Benedikt Klein (Chemistry, Marburg, 12/2019)
The surface chemical bond of non-alternant aromatic molecules on metal surfaces

52 Andrea Huttner, née Karthäuser (Physics, Marburg, 12/2019)
Kontrolle molekularer Heterostrukturen durch anorganische Template und organische Pufferschichten für optoelektronische Grenzflächenstudien

Ongoing Dissertations

53 Marleen Axt (Physics, Marburg)
Temperature-dependent pump-probe experiments by means of SHG microscopy at two-dimensional semiconductor heterostructures

54 Jürgen Belz (Physics, Marburg)
3D atom counting: antiphase boundaries in GaP

55 Tamam Bohamud (Physics, Marburg)
Non-equilibrium processes at adsorption of organic molecules on silicon

56 Natalie Dehnhardt (Chemistry, Marburg)
Complex halogenido metalates of group 15 – structure, properties and new functionalities

57 Pierre Dombrowski (Physics, Marburg)
STM/NEXAFS investigation on acene heterostructures and interfaces with TMDCs

58 Lukas Eschmann (Physics, Münster)
Interface states between metals and organic adsorbates

59 Melanie Fey (Physics, Gießen)
Charge-transfer excitations in molecular heterostructures

60 Saleh Firoozabadi (Physics, Marburg)
Transmission electron microscopy characterization of vertical hetero structures aiming for single photon detectors

61 Sebastian Flade (Physics, Marburg)
Vibrational spectroscopy of interface modes in organic heterolayer systems

62 Markus Franke (Physics, Jülich)
Geometric structure and electronic properties of hetero-molecular adsorbates on metal surfaces

63 Eugenie Geringer (Chemistry, Marburg)
Synthesis and application of a library of cluster and organic interface precursors as base for the cluster decoration with redox-active complexes and/or with metal atom/ion sequestrating macrocycles

64 Steffen Giesen (Chemistry, Marburg)
Study of intermolecular interactions in a non-orthogonal product wave function approach

65 Anna-Katharina Hansmann (Chemistry, Marburg)
Theoretical study of electronic and vibronic effects in model systems for organic interfaces

66 Julian Heep (Physics, Gießen)
Reaction mechanisms of organic molecules on Si(001)

67 Damien Heimes (Physics, Marburg)
Modelling crystal structures and electron scatter

68 Thilo Hepp (Physics, Marburg)
MOVPE on novel type-II material systems, e.g. (GaIn)(AsBi)

69 Jan Herritsch (Chemistry, Marburg)
Adsorption and reactions of tetrapyrrole complexes on single crystal surfaces

70 Nico Hofeditz (Physics, Marburg)
Time-resolved spectroscopy on organic interfaces

71 Philipp Hofmann (Chemistry, Marburg)
Synthesis of azapentacenes and substituted cyclooctynes

72 Stefan R. Kachel (Chemistry, Marburg)
Investigations on the interactions of aromatic organic compounds on metal surfaces

73 Niklas Klangwart (Chemistry, Marburg)
Synthesis of spirocyclooctynes

74 Philip Klement (Physics, Gießen)
Optical spectroscopy on 2D materials

75 Michael Kothe (Physics, Marburg)
Growth and structure of crystalline phthalocyanine thin-films

76 Claudio Krug (Chemistry, Marburg)
Investigation of reactive metal/organic interfaces

77 Jannik Lehr (Physics, Marburg)
Epitaxial growth and characterization of GaAs-based type-II W-quantum well heterostructures and lasers

78 You-Ron Lin (Physics, Jülich)
Structure of heteroepitaxial stacks of weakly interacting 2D materials and molecular layers

79 Jan-Niclas Luy (Chemistry, Marburg)
Structure and dynamics of hybrid interfaces

80 Philipp Marauhn (Physics, Münster)
Depth-dependency of the fundamental gap at the TMDC-surface

81 Oliver Maßmeyer (Physics, Marburg)
RAS-analysis of III/V-semiconductors for the preparation of specific GaP- and GaN-type interface-structures

82 Lars Meckbach (Physics, Marburg)
Linear and nonlinear optical properties of transition metal dichalcogenide monolayers and heterostructures

83 Jannick Meinecke (Chemistry, Marburg)
On the chemistry of functionalized cyclooctynes

84 Ingo Meyenburg (Physics, Marburg)
Optical spectroscopy on organic-inorganic hybrid structures

85 Lasse Münster (Physics, Marburg)
Time-resolved photoelectron spectroscopy on transition metal dichalcogenide heterostructures

86 Miriam Raths (Physics, Jülich)
Growth, structure and electronic properties of 2D-materials in SiC- and metal surfaces

87 Philipp-Henrik Richter (Physics, Marburg)
Optical spectroscopy on type-II structures with strong THz pulses

88 Luise Rost (Physics, Marburg)
Optical spectroscopy on novel III-V-semiconductors

89 Felix Schäfer (Physics, Gießen)
Ultrafast relaxation dynamics in type-II heterostructures

90 Maik Schöniger (Chemistry, Marburg)
Calorimetric measurements at interfaces

91 Matthias Tripp (Chemistry, Marburg)
On the chemistry of fluorinated pentacene and azapentacene

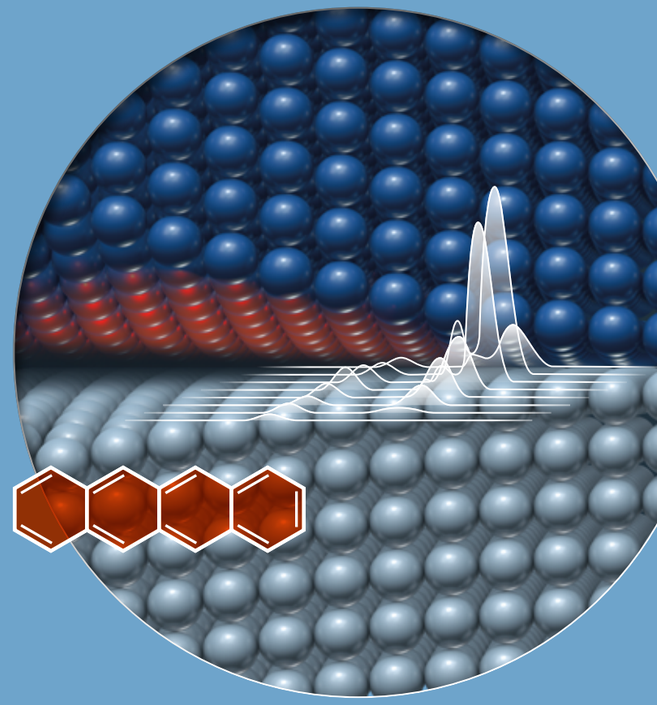
92 Bettina Wagner (Chemistry, Marburg)
Exfoliation of BiI_3 and other 2D materials and the use of porphyrin diacids as functional cations for p-block halogenido metalates

93 Maria Weseloh (Physics, Marburg)
Microscopic modeling of novel semiconductor heterostructures

94 Felix Widdascheck (Physics, Marburg)
Molecular contact-primers for improved energy-level alignment and reduced contact resistance

95 Jonas E. Zimmermann (Physics, Marburg)
Investigation of nonlinear optical effects at 2D materials

SCIENCE COMMUNICATION



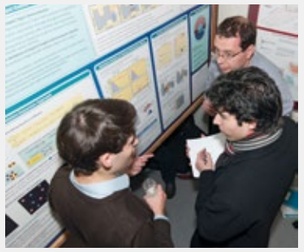
Kick-Off Meeting

27.11.–29.11.2013 – Philipps-Universität Marburg

77 participants

Speakers

- Tobias Breuer (Marburg)
- Kristina Brixius (Marburg)
- Sangam Chatterjee (Marburg)
- Stefanie Dehnen (Marburg)
- Michael Dürr (Gießen)
- Michael Gottfried (Marburg)
- Katharina Gries (Marburg)
- Wolfram Heimbrodt (Marburg)
- Kunie Ishioka (NIMS, Tsukuba, Japan)
- Peter Jakob (Marburg)
- Stephan W. Koch (Marburg)
- Ulrich Koert (Marburg)
- Peter Koval (DIPC, San Sebastián, Spain)
- Martin Liebold (Marburg)
- Gerson Mette (Univ. Zürich, Switzerland)
- Andreas Namgalies (Marburg)
- Ilya Nechaev (DIPC, San Sebastián, Spain)
- Arash Rahimi-Iman (Marburg)
- Wolfgang Stolz (Marburg)
- Ralf Tonner (Marburg)
- Kerstin Volz (Marburg)
- Gregor Witte (Marburg)



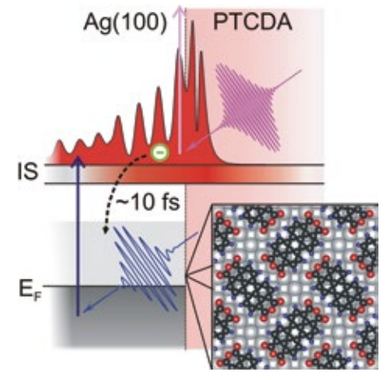
SFB Workshop on Organic / Metal Interfaces

17.07.2014 – Philipps-Universität Marburg

40 participants

Lectures

- Stefan Tautz (Jülich)
  Towards an atomistic understanding of molecule-metal-interfaces
- Peter Jakob (Marburg)
  Dynamic charge transfer processes at organic-metal interfaces
- Michael Gottfried (Marburg)
  Reactions at metal-organic interfaces
- Toshiaki Munakata (Osaka, Japan)
  Unoccupied states of organic films observed by 2PPE and STM
- Ulrich Höfer (Marburg)
  Organic/metal interface state formation
- Satoshi Kera (Okazaki, Japan)
  Violation of sudden approximation at molecular monolayer interface
- Nikolai Zaitsev (Marburg/San Sebastián)
  Adsorption geometry and electronic structure of NTCDA/Ag(111): DFT-vdW calculations with the use of localized basis set



Formation of an organic/metal interface state from Shockley resonance
Reprinted with permission from M.C.E. Galbraith, M. Marks, R. Tonner, U. Höfer, J. Phys. Chem. Lett. **5**, 50 (2014). Copyright 2014 American Chemical Society.

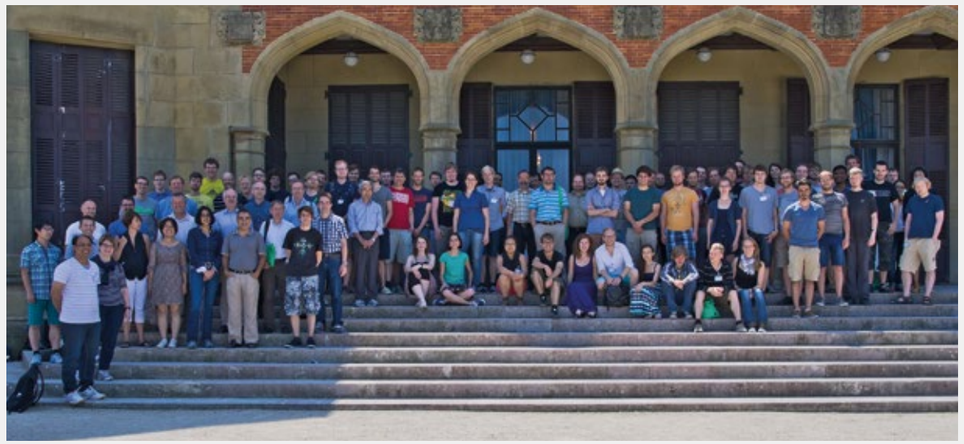
International Summer School on Semiconductor Interfaces: Methods and Model Systems

28.07.–30.07.2014 – Palacio de Miramar, San Sebastián, Spain

106 participants
Organizers: Daniel Sanchez-Portal (DIPC, San Sebastián, Spain), Kerstin Volz (Marburg)

Lectures

- Andrés Arnau (Donostia International Physics Center, San Sebastián, Spain)
  Electronic properties of molecular overlayers on surfaces
- Michael Dürr (Justus-Liebig-Universität Gießen)
  Reactions of organic molecules on semiconductor surfaces – part I: mechanisms
- Tony Heinz (Columbia University, New York, USA)
  Electronic and optical properties of atomically thin 2D materials
- Leeor Kronik (Weizmann Institute of Science, Rehovot, Israel)
  Understanding organic/inorganic interfaces from first principles
- Thomas Kuech (University of Wisconsin, Madison, USA)
  Epitaxial formation of multilayer structures: the interplay of thermodynamics, kinetics and growth behavior
- Susanne Stemmer (University of California, Santa Barbara, USA)
  Quantitative scanning transmission electron microscopy
- Gregor Witte (Philipps-Universität Marburg)
  Principles of organic thin film growth
- Wilfried Wurth (Deutsches Elektronen-Synchrotron, Hamburg)
  X-ray spectroscopy – a great toolbox for the study of interfaces
- Xiaoyang Zhu (Columbia University, New York, USA)
  Excitons at organic semiconductor interfaces



Lecturers

Andrés Arnau *(UPV/EHU and DIPC San Sebastián, Spain)*
Michael Dürr *(University of Giessen, Germany)*
Tony Heinz *(Columbia University, New York, USA)*
Leeor Kronik *(Weizmann Institute, Israel)*
Thomas Kuech *(University of Wisconsin, Madison, USA)*
Susanne Stemmer *(UC, Santa Barbara, USA)*
Gregor Witte *(University of Marburg, Germany)*
Wilfried Wurth *(DESY/University of Hamburg, Germany)*
Xiaoyang Zhu *(Columbia University, New York, USA)*

Venue

Palacio de Miramar, *San Sebastián*

For more information, please visit
www.internal-interfaces.de/summerschool2014

For registration, please e-mail
interfaces2014@dipc.org

Organizers

Dr. Daniel Sánchez-Portal
(CSIC-UPV/EHU and DIPC San Sebastián, Spain)

Prof. Dr. Kerstin Volz
(University of Marburg, Germany)

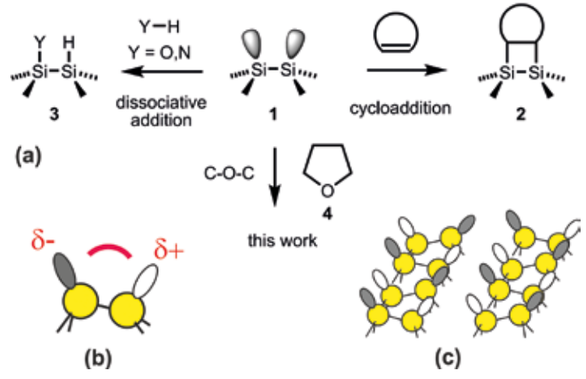
SFB 1083 Structure and Dynamics of Internal Interfaces
DFG
GRK 1782 Functionalization of Semiconductors

SFB Workshop on Interface Chemistry

18.12.2014 – Philipps-Universität Marburg

Invited Speaker

- Frank Würthner (Julius-Maximilians-Universität Würzburg)



Complex surface chemistry of an otherwise inert solvent molecule: Tetrahydrofuran on Si(001)
Reprinted with permission from G. Mette, M. Reutzel, R. Bartholomäus, S. Laref, R. Tonner, M. Dürr, U. Koert, U. Höfer, ChemPhysChem **15**, 3724 (2014). Copyright 2014 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

SFB Student Winter Seminar

08.02–12.02.2015 – Marburger Haus, Kleinwalsertal

28 participants
17 talks
11 posters

SFB Principal Investigators' Retreat

19.11.–20.11.2015 – Schloss Rauischholzhausen

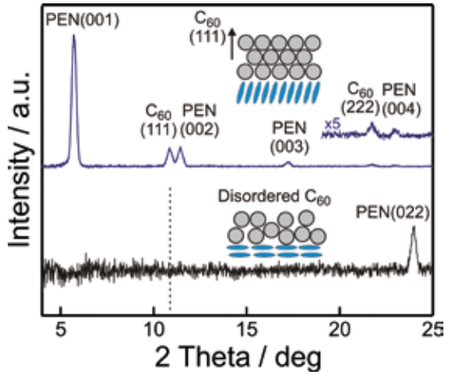
15 PIs, 6 guests, 24 talks

SFB Workshop on Organic/Organic Interfaces

12.05.2016 – Philipps-Universität Marburg

Invited Speaker

- Alexander Hinderhofer (Eberhard Karls Universität Tübingen)



Effects of molecular orientation in acceptor-donor interfaces between pentacene and C_{60} and Diels-Alder adduct formation at the molecular interface
Reprinted with permission from T. Breuer, A. Karthäuser, G. Witte, Adv. Mater. Interfaces **3**, 1500452 (2016). Copyright 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

International Conference on Internal Interfaces ICII-2016

31.05.–03.06.2016 – Philipps-Universität Marburg

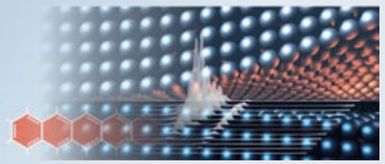
120 participants
19 invited + 16 contributed talks, 80 posters

Organizers: Ulrich Höfer, Gerson Mette, Michael Gottfried

Internal Interfaces 2016

31.05.-03.06. in Marburg

Interfaces between solids play a decisive role in modern materials sciences and their technological applications. The international conference "Internal Interfaces ICII-2016" provides an expert forum for the discussion of recent progress as well as of experimental and theoretical challenges in basic research of solid/solid interfaces. The conference will include invited talks, contributed talks and posters in a single-session format.



Venue: Philipps-Universität Marburg, Renthof
Abstract deadline: 15.04.2016

For more information please visit:
www.internal-interfaces.de/ICII-2016

Scientific Topics

- Organic/inorganic interfaces
- Organic donor/acceptor interfaces
- Type-II semiconductor interfaces
- Interfaces of 2D semiconductors
- Interfaces of topological materials
- Charge transfer processes at interfaces
- Properties of interface excitons
- Chemical reactivity & interphase formation
- Electronic & structural characterization of solid/solid interfaces
- Advances in theoretical methods for solid/solid interfaces
- Interface-specific optical spectroscopies

Invited Speakers

Friedhelm **Bechstedt**, Jena
Torsten **Fritz**, Jena
Francisco **Guinea**, Madrid
James **Hone**, New York
Bo **Iversen**, Aarhus
Norbert **Koch**, Berlin
Steven **Louie**, Berkeley
Martin **Aeschlimann**, Kaiserslautern
Yoshiyasu **Matsumoto**, Kyoto
Toshiaki **Munakata**, Osaka
Hrvoje **Petek**, Pittsburgh
Henning **Riechert**, Berlin
Michael **Rohlfing**, Münster
Julia **Stähler**, Berlin
Xiaoyang **Zhu**, New York

Organizers

Ulrich Höfer, Gerson Mette,
Michael Gottfried

SFB 1083
Structure and Dynamics of Internal Interfaces

Photos: Physics Dept., Univ. Marburg

SFB Student Winter School

17.01.–18.01.2017 – Schloss Rauischholzhausen

50 participants
10 invited talks, 18 posters

Lectures

- Ellen Backus (Max-Planck-Institute For Polymer Research, Mainz)
  Towards understanding the mechanism of water splitting on TiO_2
- Alexey Chernikov (Universität Regensburg)
  Exciton physics of semiconducting 2D materials
- Matteo Gatti (Synchrotron SOLEIL, Gif-sur-Yvette, France)
  Exciton band structure in two-dimensional materials
- Christian Papp (Friedrich-Alexander-Universität Erlangen-Nürnberg)
  In-situ studies of the reactivity of model catalysts: surface chemistry from flat surfaces to nanoparticles (part I + II)
- Katrin Siefermann (Leibniz Institute of Surface Engineering, Leipzig)
  Ultrafast photoemission electron microscopy in materials science

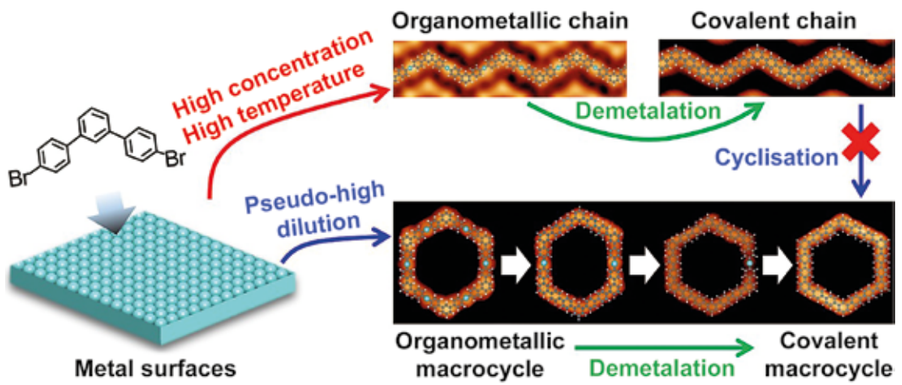
SFB Workshop on Chemical Reactions at Interfaces

02.05.2017 – Philipps-Universität Marburg

80 participants

Lectures

- Michael Dürr (Justus-Liebig-Universität Gießen)
  Reaction Dynamics of Organic Molecules on Silicon – a Route Towards Controlled Functionalization of Silicon Surfaces
- Maki Kawai (Institute for Molecular Science, Okazaki, Japan)
  Chemical Reactions at Surfaces: Single Molecular View
- Sabine Maier (Friedrich-Alexander Universität Erlangen-Nürnberg)
  On-Surface Synthesis And Electronic Properties of Molecular Networks
- Martin Schmid (Philipps-Universität Marburg)
  Reactive Metal/Organic Interfaces Studied With Hard X-ray Photoelectron Spectroscopy
- Stefan Tautz (Forschungszentrum Jülich)
  A Chemically Driven Quantum Phase Transition in a Two-Molecule Kondo System



On-Surface Pseudo-High-Dilution Synthesis of Macrocycles: Principle and Mechanism
Reprinted with permission from Q. T. Fan, T. Wang, J. Dai, J. Kuttner, G. Hilt, J. M. Gottfried, J. F. Zhu, ACS Nano **11**, 5070 (2017). Copyright 2017 American Chemical Society

Kick-Off Meeting 2nd Funding Period

06.07.2017 – Philipps-Universität Marburg

150 participants

Prof. Dr. Dr. h. c. mult. Pedro M. Echenique from the Donostia International Physics Center in San Sebastián (Spain), who contributed to the success of the first funding period as a principal investigator in former guest project GP1, gave a public presentation on "The sublime utility of useless science" and how science and innovation stand at the center of any successful strategy for the long-term economic development of a country, and how it is even more important and profitable to create an atmosphere for fundamental research rather than to define specific targets.

Invited Speaker

- Pedro Echenique (Donostia International Physics Center, San Sebastián, Spain)

SFB Workshop on Internal Interfaces – Perspectives and Challenges for Theory

08.11.2017 – Philipps-Universität Marburg

17 participants
10 posters

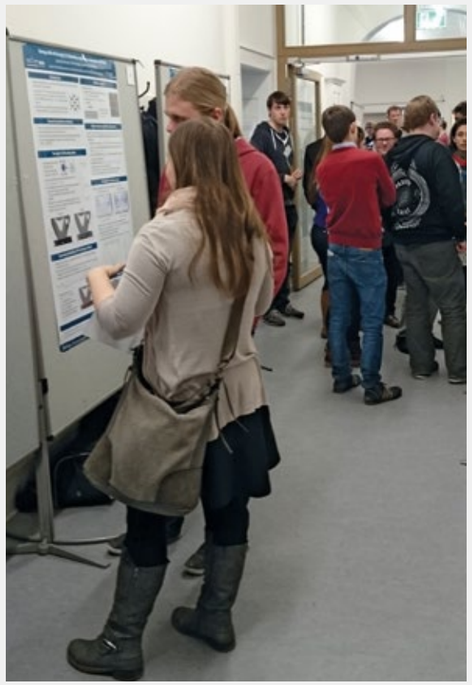
Lectures

- Frank Ortmann (Technische Universität Dresden)
  Organic Semiconductors and Interfaces: Fundamentals for Applications
- Claudia Rödl (Friedrich-Schiller-Universität Jena)
  Electronic Excitations in Matter from First Principles: From 3D towards 2D Systems
- Stefan Wippermann (Max-Planck-Institut für Eisenforschung, Düsseldorf)
  Light-Matter Interactions at Interfaces: From Analysis Techniques to Applications in Solar Energy Conversion
- Stefan Schulz (Tyndall National Institute, Cork, Ireland)
  Carrier localization effects in III-N alloys and heterostructures: Impact of random alloy fluctuations and interface roughness

SFB Student Poster Day "Meet and Greet"

01.03.2018 – Philipps-Universität Marburg

44 participants
32 posters

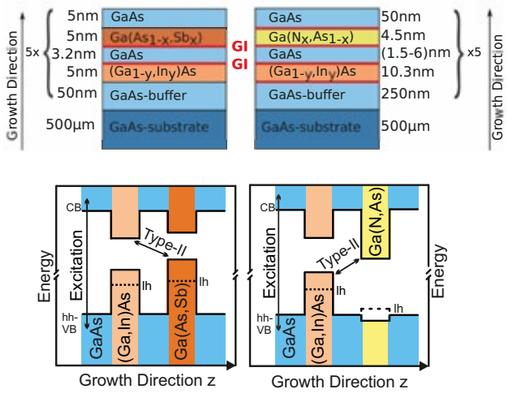


SFB Workshop on Type-II Heterostructures

17.05.2018 – Philipps-Universität Marburg

Invited Speaker

- Joachim Wagner (Fraunhofer Institute for Applied Solid State Physics, Freiburg)



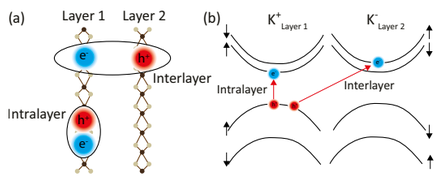
The schematic depiction show the sample structure and the band structure of the two material systems. On the left is illustrated a (Ga,In)As/Ga(As,Sb) and on the right a (Ga,In)As/Ga(N,As)-based type-II heterostructure.

SFB Workshop on TMDC Interfaces

14.06.–15.06.2018 – Westfälische Wilhelms-Universität Münster

Speakers

- François Bocquet (Jülich)
- Philipp Eickholt (Münster)
- Lukas Eschmann (Münster)
- You-Ron Lin (Jülich)
- Philipp Marauhn (Münster)
- Lars Meckbach (Marburg)
- Gerson Mette (Marburg)
- Doris Reiter (Münster)
- Christian Schwermann (Münster)
- Tineke Stroucken (Marburg)
- Steffen Michaelis de Vasconcellos (Münster)
- Robert Wallauer (Marburg)



Observation of interlayer excitons in $MoSe_2$ single crystals
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Joint Seminar GRK 1782 & SFB 1083

02.09.–06.09.2018 – Kloster Volkenroda

83 participants
41 talks, 21 posters

Session Overview

- Semiconductor Heterointerfaces I + II + III
- Metal-Organic Interfaces I + II
- Interface Excitons
- Semiconductor-Organic Interfaces
- Interface Reactions
- Transition Metal Dichalcogenides
- Novel Precursors and Nanomaterials
- Semiconductor Laser Structures

ASOMEA-9 Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications

23.10.–26.10.2018 – Hotel "4 Jahreszeiten am Schluchsee"

80 participants
19 invited + 11 contributed talks, 48 posters

Organizers: Ulrich Höfer (Marburg), Norbert Koch (Berlin)

The series of biannual ASOMEA-workshops began in 2001 as a meeting of Swedish and Japanese scientists working with spectroscopic techniques and theoretical modeling for a better understanding of organic electronic materials and related interfaces. In 2016 the scope of the workshop was widened to include the German community and the intention to focus on organic materials at advanced stages, in situ/operando techniques, and time-resolved spectroscopy to name just a few. The meeting in 2018 was therefore the first in the series to convene in Germany. Jointly organized with SFB 951 HIOS Berlin, the meeting attracted more than 80 participants from Europe, Asia and America.

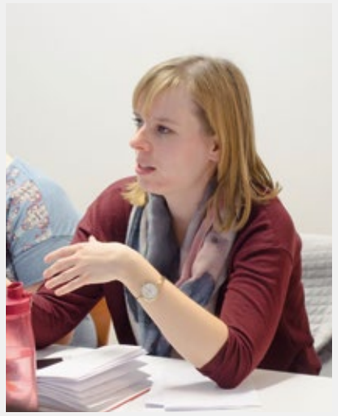
Scientific Topics

- Spectroscopy of Molecular Liquids, Solids and Interfaces
- UV and X-ray Photoelectron Spectroscopies/Microscopies
- X-ray Absorption and Emission Spectroscopies
- Time-resolved/Multi-colored Spectroscopies
- Ambient Pressure/Operando Spectroscopies
- and more

SFB Student Winter Seminar

17.02.–21.02.2019 – Marburger Haus, Kleinwalsertal

31 participants
16 talks, 15 posters



SFB Principal Investigators' Retreat

10.04.–12.04.2019 – Weinbergschlösschen Oberheimbach

19 PIs, 3 guests, 24 talks

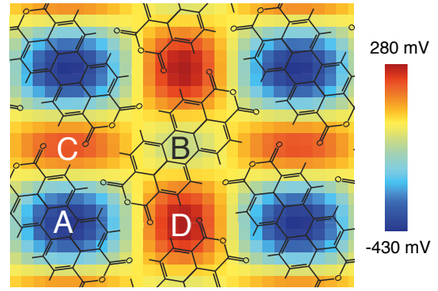
SFB Workshop on Organic Interfaces

23.05.–24.05.2019 – Forschungszentrum Jülich

35 participants
14 talks, 9 posters

Speakers

- Sangam Chatterjee (Gießen)
- Pierre Dombrowski (Marburg)
- Lukas Eschmann (Marburg)
- Qitang Fan (Marburg)
- Michael Gottfried (Marburg)
- Anna Hansmann (Marburg)
- Julian Heep (Gießen)
- Philipp Hofmann (Marburg)
- Peter Jakob (Marburg)
- Christian Kumpf (Jülich)
- Masahiro Shibuta (Marburg)
- Moritz Sokolowski (Univ. Bonn)
- Klaus Stallberg (Marburg)
- Ruslan Temirov (Jülich)



Lateral scattering potential of the PTCDA/Ag(111) interface state. Reprinted figure with permission from A. Sabitova, R. Temirov, F.S. Tautz, Phys. Rev. B **98**, 205429 (2018). Copyright 2018 by the American Physical Society.

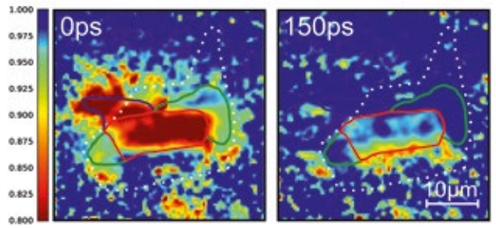
SFB Workshop on Quantum Materials

16.10.2019 – Philipps-Universität Marburg

13 participants
10 talks

Speakers

- Gustav Bihlmayer (Jülich)
- François Bocquet (Jülich)
- Sangam Chatterjee (Gießen)
- Johanna Heine (Marburg)
- Michael Heuken (RWTH Aachen)
- Philipp Marauhn (Münster)
- Gerson Mette (Marburg)
- Arash Rahimi-Iman (Marburg)
- Tineke Stroucken (Marburg)
- Robert Wallauer (Marburg)



Time-resolved second-harmonic generation of a TMDC heterostructure (red) consisting of WSe_2 (green) and $MoSe_2$ (blue) for two different times after optical excitation.

“Winter School on Ultrafast Processes in Condensed Matter” (WUPCOM)

2015, 2018, 2020 – Winklmoosalm

The informal WUPCOM workshop covers experimental and theoretical work on ultrafast phenomena in solids, heterostructures and nanoscale materials. It takes place every two or three years in the Bavarian alps. A particular focus is time-resolved photoelectron spectroscopy.

SFB 1083 invited speakers

- **WUPCOM’15** – 01.03.–06.03.2015
  Michael Horn-von Hoegen (Universität Duisburg-Essen)
  Electron diffraction at surfaces: by now ultrafast!
- **WUPCOM’18** – 04.03.–09.03.2018
  Ermin Malic (Chalmers, Gothenburg, Sweden)
  Dark exciton dynamics in atomically thin 2D nanomaterials
- **WUPCOM’20** – 08.03.–13.03.2020
  Alexander Holleitner (TU München)
  Femtosecond on-chip electronics

International Symposium on “Ultrafast Surface Dynamics” (USD-10)

11.06.–16.06.2017 – Kritische Akademie, Inzell

This bi-annual international symposium took place for the first time in 1997 and has since then been held in various locations in Europe, the USA and Japan. The conference focuses on ultrafast dynamical processes at surfaces and interfaces of solid materials and comprises electron, vibrational and magnetic dynamics on femtosecond, picosecond, and attosecond time scales. In 2017, a special anniversary session celebrated the 10th occasion of the symposium and the 60th birthday of two of its first organizers, Martin Aeschlimann and Ulrich Höfer.

SFB 1083 invited speakers

- Rupert Huber (Universität Regensburg)
- Kenta Kuroda (University of Tokyo, Japan)
- Toshiaki Munakata (Osaka University, Japan)
- Yoshiyasu Matsumoto (Kyoto University, Japan)
- Hrvoje Petek (University of Pittsburgh, USA)
- Jin Zhao (USTC, Hefei, China)

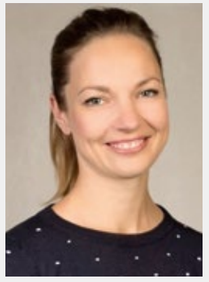
Meeting Series “From the Witches Cauldrons in Materials Science“

April 2009–2018 – Goslar

From 2009 to 2018 Prof. Dr. Katharina Al-Shamery from the Center of Interface Science in Oldenburg organized an annual conference for the last day of April, known as “Walpurgisnacht“ in the Harz mountains. “From the witches cauldrons in materials science” took place at the Rammelsberg mine, a world cultural heritage near Goslar. SFB 1083 financially supported this meeting since 2013 from its gender equality funds by inviting eminent female scientists working in the field of material sciences and interfaces, particularly from overseas. These renowned colleagues, who successfully combined family and scientific career, serve as role models for young female scientists. In contrast to large conferences the relaxed atmosphere of the small “witches” meeting ensured that young researchers could not only present their work to leaders in their fields but also discuss freely the particular challenges they face by choosing an academic career in material sciences.

Talat Rahman

Ursula Keller



Julia Stähler

Anne L’Huillier

Dagmar Gerthsen

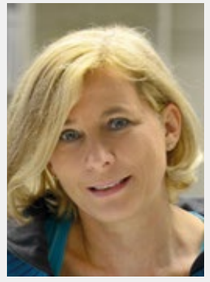
SFB 1083 invited speakers

- Claudia Draxl (Humboldt-Universität zu Berlin, 2014)
  Computational Materials Design: Modern Alchemy?
- Stefanie Dehnen (Philipps-Universität Marburg, 2014)
  The Right Concoction? How to Assemble Multinary Metallates and Intermetalloid Clusters
- Stacey F. Bent (Stanford University, Palo Alto, USA, 2015)
  The Role of Interface Engineering in Next Generation Photovoltaics
- Talat S. Rahman (University of Central Florida, Orlando, USA, 2015)
  Reactivity of Oxide and Sulfide Supported Metal Nanoparticles: Role of the Interface
- Maki Kawai (Institute for Molecular Science, Okazaki, Japan, 2017)
  Spectroscopy for Individual Molecules at Work: Action Spectroscopy using STM

Stacey Bent

Maki Kawai

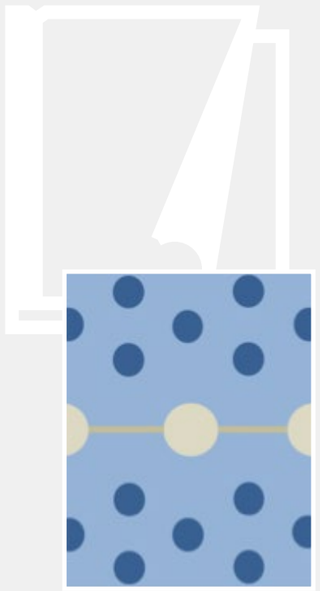
Stefanie Dehnen



Claudia Draxl

Kunie Ishioka

Special Volume on Internal Interfaces



Journal of Physics
Condensed Matter

(Guest editors: Michael Gottfried and Ulrich Höfer)

This special issue presents an up-to-date overview of research on internal interfaces of solid materials. 15 out of a total of 31 articles orginate from prinicple investigators of SFB 1083 and their collaborators. They report on a wide variety of interface-related phenomena, ranging from electronic and geometric structure over electron transfer dynamics to diffusion processes and chemical reactions at interfaces. The publications address fundamental as well as applied aspects of different classes of heterostructures, from ultrathin bilayer structures to buried bulk interfaces.

J.M. Gottfried, U. Höfer
Preface: fresh perspectives on internal interfaces
Journal of Physics: Condensed Matter **31**, 500301 (2019).

N.L. Zaitsev, P. Jakob, R. Tonner
Structure and vibrational properties of the PTCDA/Ag(111) interface: bilayer versus monolayer
Journal of Physics: Condensed Matter **30**, 354001 (2018).

L. Meckbach, U. Huttner, L. Bannow, T. Stroucken, S.W. Koch
Interlayer excitons in transition-metal dichalcogenide heterostructures with type-II band alignment
Journal of Physics: Condensed Matter **30**, 354002 (2018).

W.-D. Zabka, M. Mosberger, Z. Novotny, D. Leuenberger, G. Mette, T. Kälin, B. Probst, J. Osterwalder
Functionalization and passivation of ultrathin alumina films of defined sub-nanometer thickness with self-assembled monolayers
Journal of Physics: Condensed Matter **30**, 424002 (2018).

K. Brixius, A. Beyer, G. Mette, J. Güdde, M. Dürr, W. Stolz, K. Volz, U. Höfer
Second-harmonic generation as probe for structural and electronic properties of buried GaP/Si(001) interfaces
Journal of Physics: Condensed Matter **30**, 484001 (2018).

T.R. Kafle, B. Kattel, T. Wang, W.-L. Chan
The relationship between the coherent size, binding energy and dissociation dynamics of charge transfer excitons at organic interfaces
Journal of Physics: Condensed Matter **30**, 454001 (2018).

A. Lerch, J.E. Zimmermann, A. Namgalies, K. Stallberg, U. Höfer
Two-photon photoemission spectroscopy of unoccupied electronic states at CuPc/PTCDA/Ag(111) interfaces
Journal of Physics: Condensed Matter **30**, 494001 (2018).

C. Länger, J. Heep, P. Nikodemiak, T. Bohamud, P. Kirsten, U. Höfer, U. Koert, M. Dürr
Formation of Si/organic interfaces using alkyne-functionalized cyclooctynes – precursor-mediated adsorption of linear alkynes versus direct adsorption of cyclooctyne on Si(001)
Journal of Physics: Condensed Matter **31**, 034001 (2019).

L. Rost, S. Gies, M. Stein, C. Fuchs, S. Nau, W. Stolz, M. Koch, W. Heimbrodt
Correlation of Optical Properties and Interface Morphology in Type-II Semiconductor Heterostructures
Journal of Physics: Condensed Matter **31**, 014001 (2019).

T. Breuer, T. Geiger, H. Bettinger, G. Witte
Diels-Alder Adduct Formation at Solid Interfaces between Fullerenes and Acenes
Journal of Physics: Condensed Matter **31**, 034003 (2019).

A. Stein, D. Rolf, C. Lotze, C. Czekelius, K.J. Franke, P. Tegeder
Electronic structure of an iron porphyrin derivative on Au(111)
Journal of Physics: Condensed Matter **31**, 044002 (2019).

T. Yamada, N. Kawakita, C. Okui, T. Munakata
Hybridization of an unoccupied molecular orbital with an image potential state at a lead phthalocyanine/graphite interface
Journal of Physics: Condensed Matter **31**, 044004 (2019).

M.H. Futscher, T. Schultz, J. Frisch, M. Ralaiarisoa, E. Metwalli, M.V. Nardi, P. Müller-Buschbaum, N. Koch
Electronic properties of hybrid organic/inorganic semiconductor pn-junctions
Journal of Physics: Condensed Matter **31**, 064002 (2019).

S. Vempati, J.-C. Deinert, L. Gierster, L. Bogner, C. Richter, N. Mutz, S. Blumstengel, A. Zykov, S. Kowarik, Y. Garmshausen
Uncovering the (un-)occupied electronic structure of a buried hybrid interface
Journal of Physics: Condensed Matter **31**, 094001 (2019).

M. Schmid, S.R. Kachel, B.P. Klein, N. Bock, P. Müller, R. Riedel, N. Hampp, J.M. Gottfried
Reactive Metal-Organic Interfaces Studied with HAXPES: Controlled Formation of Metalloporphyrin Interphase Layers During Metal Vapor Deposition onto Porphyrin Films
Journal of Physics: Condensed Matter **31**, 094002 (2019).

K. Ishioka, A. Beyer, W. Stolz, K. Volz, H. Petek, U. Höfer, C. Stanton
Coherent optical and acoustic phonons generated at lattice-matched GaP/Si(001) heterointerfaces
Journal of Physics: Condensed Matter **31**, 094003 (2019).

M. Rahaman, C. Wagner, A. Mukherjee, A. Lopez-Rivera, S. Gemming, D.R.T. Zahn
Probing interlayer excitons in a vertical van der Waals p-n junction using a scanning probe microscopy technique
Journal of Physics: Condensed Matter **31**, 114001 (2019).

J. Felter, J. Wolters, F. Bocquet, F.S. Tautz, C. Kumpf
Momentum microscopy on the micrometer scale: Photoemission micro-tomography applied to single molecular domains
Journal of Physics: Condensed Matter **31**, 114003 (2019).

H. Sun, Q. Zheng, W. Lu, J. Zhao
Ultrafast dynamics of solvated electrons at anatase TiO_2/H_2O interface
Journal of Physics: Condensed Matter **31**, 114004 (2019).

D. Becker-Koch, B. Rivkin, F. Paulus, H. Xiang, Y. Dong, Z. Chen, A.A. Bakulin, Y. Vaynzof
Probing charge transfer states at organic and hybrid internal interfaces by photothermal deflection spectroscopy
Journal of Physics: Condensed Matter **31**, 124001 (2019).

A. Alekhin, I. Razdolski, M. Berritta, D. Bürstel, V. Temnov, D. Diesing, U. Bovensiepen, G. Woltersdorf, P.M. Oppeneer, A. Melnikov
Magneto-optical properties of Au upon the injection of hot spin-polarized electrons across Fe/Au(001) interfaces
Journal of Physics: Condensed Matter **31**, 124002 (2019).

S.B. Srivastava, M.H. Modi, S.K. Ghosh, S.P. Singh
Investigation of the buried planar interfaces in multi-layered inverted organic solar cells using X-ray reflectivity and impedance spectroscopy
Journal of Physics: Condensed Matter **31**, 124003 (2019).

R. Döring, N. Rosemann, A. Huttner, T. Breuer, G. Witte, S. Chatterjee
Charge transfer processes and carrier dynamics at the pentacene – C_{60} interface
Journal of Physics: Condensed Matter **31**, 134001 (2019).

S. Thussing, L. Fernandez, P. Jakob
Thermal stability and interlayer exchange processes in heterolayers of TiOPc and PTCDA on Ag(111)
Journal of Physics: Condensed Matter **31**, 134002 (2019).

R. Forker, M. Gruenewald, F. Sojka, J. Peuker, P. Mueller, C. Zwick, T. Huempfner, M. Meissner, T. Fritz
Fraternal twins: distinction between PbPc and SnPc by their switching behaviour in a scanning tunnelling microscope
Journal of Physics: Condensed Matter **31**, 134004 (2019).

P. Farin. M. Marquardt, W. Martyanov, J. Belz, A. Beyer, K. Volz, A. Lenz
Three-dimensional structure of antiphase domains in GaP on Si(001)
Journal of Physics: Condensed Matter **31**, 144001 (2019).

R. Tsuruta, T. Hosokai, S. Yamanaka, K. Yoshida, Y. Mizuno, T. Koganezawa, Y. Nakayama
Evolution of crystallinity at a well-defined molecular interface of epitaxial C_{60} on the single crystal rubrene
Journal of Physics: Condensed Matter **31**, 154001 (2019).

D. Balle, C. Schedel, T. Chassé, H. Peisert
Interface properties of CoPc and $CoPcF_{16}$ on graphene/nickel: influence of germanium intercalation
Journal of Physics: Condensed Matter **31**, 174004 (2019).

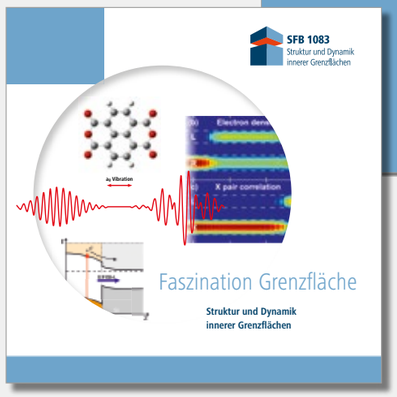
M.-T. Chen, O.T. Hofmann, A. Gerlach, B. Bröker, C. Bürker, J. Niederhausen, T. Hosokai, J. Zegenhagen, A. Vollmer, R. Rieger
Energy-level alignment at strongly coupled organic–metal interfaces
Journal of Physics: Condensed Matter **31**, 194002 (2019).

N. Zaitsev, R. Tonner, I. Nechaev
Spin-orbit split two-dimensional states of BiTeI/Au(111) interfaces
Journal of Physics: Condensed Matter **31**, 204001 (2019).

F. Edler, I. Miccoli, H. Pfnür, C. Tegenkamp
Space charge layer effects in silicon studied by in situ surface transport
Journal of Physics: Condensed Matter **31**, 214001 (2019).

Information material

- SFB 1083's image brochure in German is an introduction to its research aimed at interested students and general public. The focus is on the portraits of the participating researchers and the general idea behind the individual research performed.
- The activity report presented here highlights the research results from recent years in English and provides a scientific overview for the broader research community.



- The SFB 1083 image film takes the non-specialist on a journey down to the atomic scale and shows the progress at the forefront of research at internal interfaces. The 6-minute video clip made by Till Schürmann from Gießen is not a demanding educational film. Rather, it is a visually stunning piece that looks like science fiction straight out of the cinema, with flights through luminous molecules, with exotic excitons and room-filling laser apparatus. The film also has a very impressive soundtrack. Gustav Holst's (1874–1934) composition "The Planets" was re-orchestrated especially for this film.

Presently the film is only available in German. Visitors of Chemikum Marburg can enjoy it on a 4K OLED screen. An English version will become available soon.

Watch the film-documentary on youtube:
https://youtu.be/9-kPE0hwNMM

chemikum marburg

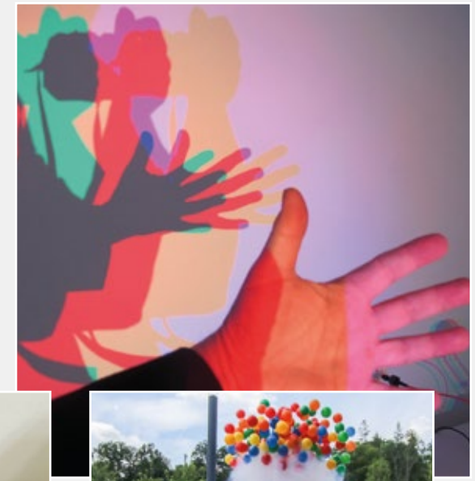
Chemikum Marburg e.V. is a successful science center and hands-on experimental laboratory in the center of the university town of Marburg. Some 13,000 visitors annually come to its premises for workshops, guided tours and presentations.

SFB 1083 with its research is now the focus of about a dozen exhibits and experiments. Overall Chemikum Marburg has set up about 50 experimental stations covering various natural science aspects of people's everyday lives. SFB experiments, for example, explain light and wave phenomena. One particular experiment includes an atomic force microscope constructed from Lego, which is able to relay surface images at a miniscule scale. Other SFB experiments, for example, focus on the role of interfaces and surfaces in smartphones, adhesion in construction, and nylon-production.

SFB experiments require a more intense supervision than is standard in classic science centers. These experiments are therefore overseen by senior or PhD-students, but importantly, the experiments itself are performed by the visitors.

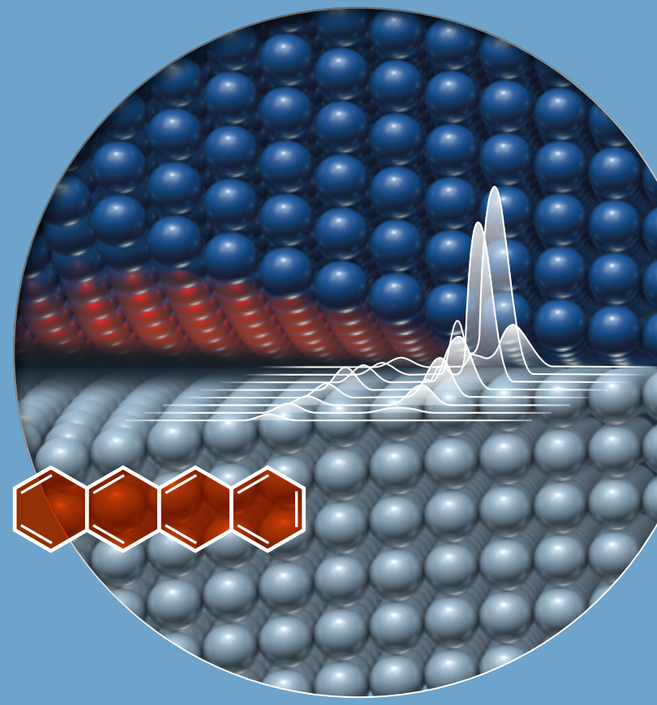
Due to its location just minutes from the train station Chemikum Marburg has a reach beyond the city's boundaries and proves attractive to visitors from Frankfurt to Kassel and even beyond. In addition, Chemikum Marburg has created a mobile setup with which it partakes in city- and street-festivals. SFB's solar cell experiment has proven a particular success while "on the road".

The SFB's experiments of course help to promote its research, but at the same time they also strengthen Chemikum Marburg as it is able to set itself apart from other science centers. Beginning in 2017 it has been offering special workshops centered on surface- and interface-related phenomena as shown in SFB 1083's specifically developed experiments. These workshops prove particularly popular with school classes and on "Girl's Day".



A hit with visitors is the SFB's postcard „Wir gehen an die Grenze!", a pun on the German term for interface, which is „innere Grenzfläche". In translation the postcard basically reads "We are going all the way to the edge!". A flyer is produced to advertise the special workshops and the SFB's image brochure is also made available as a handout.

PRINCIPAL INVESTIGATORS



Principal Investigators

Dr. François C. Bocquet (married Posseik)

Forschungszentrum Jülich (FZ Jülich), Peter Grünberg Institut (PGI-3)

f.bocquet@fz-juelich.de PI since 07/2017

Expertise: Experimental physics, surface vibron spectroscopy, electron specctroscopy, epitaxial graphene, adsorption on semiconductor and metal surfaces

University Education

2003–06	Bachelor of Science, majoring in Physics, Université Joseph Fourier, France
2006–07	Master of Science (first year), University of Birmingham, UK
2007–08	Master of Science (second year), Université Paris-Sud 11, France
2012	Doctoral degree in Physics, Aix-Marseille Université, France

Professional Experience

2011–13	Postdoc, Peter Grünberg Institut, FZ Jülich
2012	PhD thesis prize, Doct. School of Physics & Condensed Matter, Marseille, France
2013	PhD thesis prize, C'Nano PACA, France
2013–16	Helmholtz Postdoc Programme, Peter Grünberg Institut, FZ Jülich
Since 2016	Postdoc, Peter Grünberg Institut, FZ Jülich

Prof. Dr. Robert Berger

Philipps-Universität Marburg, Department of Chemistry

robert.berger@uni-marburg.de PI since 10/2015

Expertise: Quantum & theoretical chemistry, method development (vibronic structure theory, electroweak quantum chemistry) and application (incl. theoretical spectroscopy, materials, catalysis)

University Education

1993	Diploma degree in Chemistry (Dipl. Chem.), Univ. Münster
1997	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Münster

Professional Experience

1993–97	Research Assistant, Univ. Münster
1997–00	Postdoc, Laboratory of Physical Chemistry, ETH Zurich
1998–99	Postdoctoral scholarship of the German Research Foundation
2000–03	Researcher and Liebig-Fellow, TU Berlin
2003–05	Head of Junior Research Group (funded by Volkswagen Foundation), TU Berlin
2005–09	Fellow Frankfurt Inst. f. Adv. Stud., Univ. Frankfurt; Head Volkswagen Found. research group
2008	Hellmann Award of the Arbeitsgemeinschaft Theoretische Chemie
2009–14	Professor (W2) at the Clemens-Schöpf Institute, TU Darmstadt
2012	OYGA-Award, Lise Meitner-Minerva Center for Comput. Quant. Chem., Jerusalem, Israel
Since 2014	Professor (W3) for Theoretical Chemistry, Univ. Marburg

Prof. Dr. Sangam Chatterjee

Justus-Liebig-Universität Gießen, Institute of Experimental Physics I

sangam.chatterjee@physik.uni-giessen.de PI since 10/2013

Expertise: Experimental physics, semiconductor spectroscopy, ultrafast carrier dynamics, properties of lasers, characterization, and development

University Education

2000	Diploma degree in Physics (Dipl. Phys.), Universität Karlsruhe (TH)
2002	Master's degree in Optical Sciences (M.Sc.), Univ. Arizona, Tucson, AZ/USA
2003	Doctoral degree in Optical Sciences (Ph.D.), Univ. Arizona, Tucson, AZ/USA
2009	Habilitation in Experimental Physics, Univ. Marburg

Professional Experience

2000–03	Research Ass./Associate, Optical Sci. Center, Univ. Arizona, Tucson, AZ/USA
2001	State of Arizona Proposition 301 Fellowship in Quantum Electronics
2005–09	Research Associate, Faculty of Physics, Univ. Marburg
2009–16	Lecturer and Group Leader Optics, Faculty of Physics, Univ. Marburg
2010–12	Substitute Professor (W2), Faculty of Physics, Univ. Marburg
2016	Heisenberg Professorship, Univ. Gießen
Since 2016	Professor (W3), Inst. of Experimental Physics I, Univ. Gießen

Prof. Dr. Stefanie Dehnen

Philipps-Universität Marburg, Department of Chemistry

dehnen@chemie.uni-marburg.de PI since 10/2013

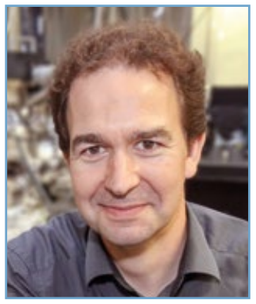
Expertise: Inorganic and organoelement cluster syntheses, X-ray diffraction, spectroscopic characterization (NMR/IR/Raman/UV-vis.), thermogravimetric analyses, molecular quantum chemistry

University Education

1993	Diploma degree in Chemistry (Dipl. Chem.), Univ. Karlsruhe
1996	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Karlsruhe
2004	Habilitation in Inorganic Chemistry, Univ. Karlsruhe

Professional Experience

1997	Feodor Lynen-Stipendium of Alexander-von-Humboldt-Stiftung
1998–03	Margarete von Wrangell-Habilitations-Stipendium (State of Baden-Württemberg)
2004	Wöhler-Nachwuchspreis from GDCh
2005	Heisenbergstipendium from DFG
Since 2006	Executive Director of Chemikum Marburg
Since 2006	Professor (W3) for Inorganic Chemistry, Univ. Marburg
Since 2016	Member of Review Board (Fachkollegium) at German Research Foundation (DFG)
2018	Prize for the Advancement of Women in Science, Univ. Marburg
Since 2018	Member of the Board of Trustees of the Verband der Chemischen Industrie (VCI)
Since 2018	Associate Editor of the journal Inorganic Chemistry
Since 2019	Chairwoman of the Wöhler-Vereinigung für Anorganische Chemie



Prof. Dr. Michael Dürr

Justus-Liebig-Universität Gießen, Institute of Applied Physics

michael.duerr@ap.physik.uni-giessen.de PI since 07/2017

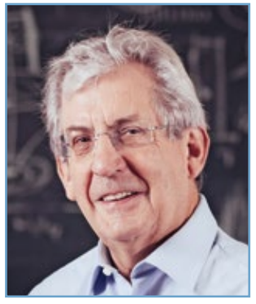
Expertise: Experimental physics, reaction dynamics on semiconductor surfaces, scanning tunneling microscopy, cluster-surface dynamics and application in mass spectrometry

University Education

1997	Diploma degree in Physics (Dipl. Phys.), TU München
2000	Doctoral degree in Physics (Dr. rer. nat.), TU München

Professional Experience

1997–98	Research Assistant, MPI for Quantum Optics, Garching
1999	Visiting Scientist, Physics Department, Columbia Univ. New York, NY/USA
2000–02	Postdoc, Univ. Marburg
2002–06	Scientist/Senior Scientist at Materials Science Laboratories, Sony Dtl., Stuttgart
2006	Visiting Scientist at Sony Materials Laboratories, Atsugi, Japan
2006	Sony Materials Laboratories Science Award, Sony Japan
2006	Sony Deutschland Patent Award, Sony Deutschland
2006–13	Professor (W2), Hochschule Esslingen
2012	Visiting professor, Peking Univ., State Key Laboratory, China
Since 2013	Professor (W2), Institute of Applied Physics, Univ. Gießen



Prof. Dr. Pedro Miguel Echenique

Donostia International Physics Center (DIPC), San Sebastián, Spain

pedromiguel.echenique@ehu.es PI 10/2013–06/2017

Expertise: Theoretical solid state physics, electronic properties of surfaces and nanostructures

University Education

1972	Bachelor in Physics (B.Sc.), Univ. Navarra, Spain
1976	Doctor of Philosophy (Ph.D.), Univ. Cambridge, UK
1977	Doctoral degree in Physics (Ph.D.), Univ. Barcelona, Spain

Professional Experience

1978–80	Professor of Solid State Physics, Univ. Barcelona, Spain
1980–83	Education Minister of the Basque Government
1983–84	Culture and Education Minister and Spokesman of the Basque Government
1984–86	Visiting Professor, Cavendish Laboratory, Univ. Cambridge, UK
Since 1986	Professor of Physics, Univ. of the Basque Country
Since 1999	President of the Donostia Int. Physics Center (DIPC), San Sebastián, Spain
2001–07	Member of the Rector's Board Spanish Center for Scientific Research
2007–12	President of Jakiunde, Basque Acad. of Sciences, Humanity and Arts
2011–19	Vice-President of Fundación Euskampus
2018	Honorary member of the European Physical Society (EPS)

Prof. Dr. Michael Gottfried

Philipps-Universität Marburg, Department of Chemistry

michael.gottfried@chemie.uni-marburg.de PI since 10/2013

Expertise: Surface chemistry, model catalysis, organic and organometallic thin films, surface coordination chemistry, photoelectron spectroscopy, nanojoule calorimetry

University Education

1999	Diploma degree in Chemistry (Dipl. Chem.), FU Berlin
2003	Doctoral degree in Chemistry (Dr. rer. nat.), Freie Universität (FU) Berlin
2009	Habilitation in Physical Chemistry, Univ. Erlangen-Nürnberg

Professional Experience

1999–03	Research Assistant, Dept. of Chemistry, FU Berlin
2003–04	Postdoc, Dept. of Chemistry, Univ. of Washington, Seattle, WA/USA
2004	Feodor-Lynen Fellowship of the Alexander von Humboldt Foundation
2004–11	Group Leader, Dept. of Chemistry and Pharmacy, Univ. Erlangen-Nürnberg
2009–11	Lecturer, Dept. of Chemistry and Pharmacy, Univ. Erlangen-Nürnberg
2010	Emmy-Noether Habilitation Prize of the Univ. Erlangen-Nürnberg
Since 2011	Professor (W2) for Physical Chemistry, Univ. Marburg
2012	Visiting Professorship of the Chinese Academy of Sciences
Since 2012	Member of the Scientific Selection Panel, Helmholtz-Zentrum Berlin / BESSY
2014	Chinese Academy of Sciences, International Collaboration Award
2016	SCS Lectureship of the Swiss Chemical Society

Dr. Katharina Gries

Philipps-Universität Marburg, Dept. of Physics, Materials Science Center (WZMW)

katharina.gries@physik.uni-marburg.de PI 10/2013-06/2017

Expertise: Experimental physics, structural analysis, transmission electron microscopy

University Education

2007	Diploma degree in Physics (Dipl. Phys.), Univ. Bremen
2011	Doctoral degree in Physics (Dr. rer. nat.), Univ. Bremen

Professional Experience

2007–11	Research Assistant, Univ. Bremen
2011–13	Postdoc, Univ. Marburg
2013–17	Research Associate, Univ. Marburg

Prof. Dr. Wolfram Heimbrodt

Philipps-Universität Marburg, Department of Physics

Wolfram.Heimbrodt@physik.uni-marburg.de PI since 10/2013

Expertise: Experimental Physics, optical and magneto-optical spectroscopy of semiconductor nanostructures, exciton dynamics, Raman-spectroscopy

University Education

1975–80	Diploma degree in Physics (Dipl. Phys.), TU Dresden
1985	Doctoral degree in Physics (Dr. rer. nat.), Humboldt Univ. Berlin
1996	Habilitation in Experimental Physics, Humboldt Univ. Berlin

Professional Experience

1980–85	Postgrad. Research Student, Inst. of Semiconductor Optics, Humboldt Univ. Berlin
1986	Humboldt Award, Humboldt Universität zu Berlin
1986–93	Postdoc. Res. Fellow, Inst. of Optics and Spectroscopy, Humboldt Univ. Berlin
1993–96	Res. Assistant and stand-in Professor, Group Leader, Humboldt Univ. Berlin
1996–97	Senior Research Fellow, Univ. of Norwich, School of Physics, UK
Since 1998	Professor (C3) for Experimental Physics, Univ. Marburg
2002	Visiting scientist, Univ. of Bath, UK
2007	Visiting scientist, Tohoku Univ., Sendai, Japan
2012	Visiting scientist, Univ. of Bath and Heriott-Watt Univ., Edinburgh, UK

Dr. Johanna Heine

Philipps-Universität Marburg, Department of Chemistry

johanna.heine@chemie.uni-marburg.de PI since 07/2017

Expertise: Inorganic synthesis, hybrid materials, X-ray diffraction, spectroscopic characterization (UV-visible/luminescence), thermogravimetric analyses

University Education

2008	Diploma degree in Chemistry (Dipl. Chem.), Univ. Marburg
2011	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Marburg

Professional Experience

2012	Postdoc-Scholarship from the State of Bavaria
2012–13	Postdoc, Univ. Würzburg
Since 2013	Junior Group Leader in Chemistry, Univ. Marburg

Prof. Dr. Ulrich Höfer

Philipps-Universität Marburg, Department of Physics

hoefer@physik.uni-marburg.de PI since 10/2013

Expertise: Experimental physics, laser spectroscopy of surfaces and interfaces, ultrafast electron dynamics, adsorption on semiconductor surfaces

University Education

1985	Diploma degree in Physics (Dipl. Phys.), TU München,
1989	Doctoral degree in Physics (Dr. rer. nat.), TU München
1996	Habilitation in Experimental Physics, TU München

Professional Experience

1990–91	Visiting Scientist, IBM Research Center, Yorktown Heights, NY/USA
1992–99	Group Leader, Max-Planck-Institut für Quantenoptik (MPQ), Garching
1995	Arnold-Sommerfeld-Prize of the Bavarian Academy of Sciences and Humanities
1996–99	Lecturer (Dozent), Dept. of Physics, TU München
Since 1999	Professor (C4/W3) for Experimental Physics, Univ. Marburg
2006	Fellow of the American Physical Society (USA)
2007–09	Dean of the Department of Physics, Univ. Marburg
2011	Ikerbasque Research Professor (Basque Country, Spain), DIPC, San Sebastián, Spain
Since 2013	Spokesman SFB 1083 "Structure and Dynamics of Internal Interfaces"
2015	Fellow of the Japanese Society for the Promotion of Science (Japan)

Prof. Dr. Heinz J. Jänsch

Philipps-Universität Marburg, Department of Physics

Heinz.jaensch@physik.uni-marburg.de PI 10/2013-06/2017

Expertise: Experimental physics, nuclear magnetic resonance of surfaces, optical pumping, infrared spectroscopy, adsorption and reaction at metal surfaces

University Education

1982	Diploma in Physics (Dipl. Phys.), Univ. Marburg
1985	Doctoral degree in Physics (Dr. rer. nat.), Univ. Marburg
1995	Habilitation in Experimental Physics, Univ. Marburg

Professional Experience

1985–87	Research Assistant, Max-Planck-Inst. for Nuclear Physics
1987–89	Postdoc, Univ. California Santa Barbara, CA/USA
1989–90	Research Associate, Pittsburgh Univ., PA/USA
Since 1990	Research Associate, Univ. Marburg
Since 2003	apl. Professor, Univ. Marburg

Prof. Dr. Peter Jakob

Philipps-Universität Marburg, Department of Physics

peter.jakob@physik.uni-marburg.de PI since 10/2013

Expertise: Experimental physics, vibrational spectroscopy of surfaces and interfaces, surface chemistry, kinetics of surface processes, organic molecular beam deposition

University Education

1985	Diploma degree in Physics (Dipl. Phys.), TU München
1989	Doctoral degree in Physics (Dr. rer. nat.), TU München
1998	Habilitation in Experimental Physics, TU München

Professional Experience

1985–89	Research Assistant, Physics-Dept. E20, TU München
1989–90	Postdoc, Max-Planck-Institut für Quantenoptik (MPQ), Garching
1990–92	DFG-stipend: Time resolved FTIR investigations of kinetic processes at surfaces
1990–92	Postdoc, AT&T Bell Laboratories, Murray Hill, NJ/USA
1992–98	Research Scientist (C1), Physics-Dept. E20, TU München
1998–02	Lecturer (Dozent) (C2), Physics-Dept. E20, TU München
Since 2002	Professor (C3) for Experimental Physics, Univ. Marburg

Prof. Dr. Mackillo Kira

Philipps-Universität Marburg, Department of Physics

mackkira@umich.edu PI 10/2013-08/2016

Expertise: Semiconductor quantum optics, quantum optics, condensed matter theory, many-body interactions, photon correlations, coherent and ultrafast phenomena

University Education

1992	Master of Science (M.Sc.), Helsinki Univ. of Technology, Finland
1996	Doctor of Technology, Helsinki Univ. of Technology, Finland

Professional Experience

1992–93	Researcher, Univ. Jyväskylä, Finland
1993–95	Reseracher, Univ. Helsinki, Finland
1996–98	Marie-Curie Postdoctoral Fellowship, Univ. Marburg
1999–02	Research Associate, Royal Institute of Physics, Stockholm, Sweden
2002	Academy Research Fellow, Adacemy of Finland
2002–06	Assistant Professor, Univ. Marburg
2006–16	Professor for Theoretical Physics, Univ. Marburg
2015	Elected Fellow of the American Physical Society (APS)
Since 2016	Professor, Univ. of Michigan, Ann Arbor, MI/USA

Prof. Dr. Martin Koch

Philipps-Universität Marburg, Department of Physics

martin.koch@physik.uni-marburg.de PI since 10/2013

Expertise: Experimental physics, laser spectroscopy of semiconductors and semiconductor heterostructures, terahertz spectroscopy

University Education

1991	Diploma degree in Physics (Dipl. Phys.), Univ. Marburg
1995	Doctoral degree in Physics (Dr. rer. nat.), Univ. Marburg

Professional Experience

1994	Feodor Lynen Scholarship by Alexander von Humboldt Foundation
1995	"The J. J. Thompson Premium" of the Inst. of Eng. and Technol., UK
1995–96	Postdoc at Bell Laboratories / Lucent Technologies, Holmdel, NJ/USA
1996–98	Research Assistant, Physics Department, Ludwig-Maximilians-Univ. München
1998–09	Professor (C3), Technical Univ. of Braunschweig
2003	Kaiser Friedrich Research Award
2003	Visiting scientist, Physics Department, Univ.of California Santa Barbara, CA/USA
Since 2007	First chairman of Deutsches Terahertz-Zentrum e.V.
2009	IPB Patent Award
Since 2009	Professor (W3) for Experimental Semiconductor Physics, Univ. Marburg

Prof. Dr. Stephan W. Koch

Philipps-Universität Marburg, Department of Physics

stephan.w.koch@physik.uni-marburg.de PI since 10/2013

Expertise: Condensed matter theory, optical and electronic semiconductor properties, many-body interactions, semiconductor quantum optics, laser theory, coherent and ultrafast phenomena

University Education

1977	Diploma degree in Physics (Dipl. Phys.), Univ. Frankfurt
1979	Doctoral degree in Physics (Dr. phil. nat.), Univ. Frankfurt
1983	Habilitation in Theoretical Physics, Univ. Frankfurt

Professional Experience

1985–86	Heisenberg Fellow (DFG), Univ. Frankfurt
1986–93	Assoc. Prof. / Prof., Univ. of Arizona, Phys. Dept. & Optical Sci. Ctr., Tucson, AZ/USA
Since 1993	Adjunct Professor, Univ. of Arizona, Optical Sciences Center, Tucson, AZ/USA
1993–19	Professor (C4/W3), Univ. Marburg
1993	Fellow of the Optical Society of America (USA)
1995–01	Speaker SFB 383 "Disorder on Mesoscopic Scales", Univ. Marburg
1997	Leibniz Prize of the Deutsche Forschungsgemeinschaft (DFG)
1999	Max-Planck Research Prize of the A. v. Humboldt Foundation & Max-Planck-Soc.
2001–06	Coordinator Interdisciplinary Res. Center "Optodynamics", Univ. Marburg
2006	Prize for the Advancement of Women in Science, Univ. Marburg
Since 2019	Senior Research Professor, Univ. Marburg

Prof. Dr. Ulrich Koert

Philipps-Universität Marburg, Department of Chemistry

koert@chemie.uni-marburg.de PI since 10/2013

Expertise: Organic synthesis of complex molecules (natural products, functional molecules, ion channels, molecular switches), development of selective and efficient synthetic methods

University Education

1985	Diploma degree in Chemistry (Dipl. Chem.), Univ. Frankfurt
1989	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Frankfurt
1994	Habilitation in Organic Chemistry, Univ. Marburg

Professional Experience

1988–90	Postdoc, Université Louis Pasteur Strasbourg, France
1990–94	Habilitand, Dept. of Chemistry, Univ. Marburg
1995	Visiting Associate Professor Univ. of Wisconsin at Madison, WI/USA
1996	Professor (C3) for Organic Chemistry, LMU München
1996–01	Professor (C4) for Organic and Bioorganic Chemistry, Humboldt Univ. Berlin
1998	Otto-Bayer Prize
2001	Steinhofer Lectureship Universität Freiburg
2001–13	Professor (C4) for Organic Chemistry, Univ. Marburg
2011	Visiting professor, Osaka-Prefecture University, Japan
2013–16	Vice-President for Research, Univ. Marburg
Since 2013	Professor (W3) for Organic Chemistry, Univ. Marburg

Prof. Dr. Christian Kumpf

Forschungszentrum Jülich (FZ Jülich), Peter Grünberg Institut (PGI-3)

c.kumpf@fz-juelich.de PI since 07/2017

Expertise: Surface and interface science, metal/organic interfaces, molecular adsorbates and nanostructures at surfaces, X-ray standing waves; electron microscopy and diffraction

University Education

1994	Diploma in Physics (Dipl. Phys.), Univ. Erlangen
1998	Doctoral degree in Physics (Dr. rer. nat.), Univ. Rostock
2006	Habilitation in Experimental Physics, Univ. Würzburg

Professional Experience

1999–01	Postdoc, Risø National Laboratory, Roskilde, Denmark
2001–06	Research Assistent (C1), Univ. Würzburg
2006–08	Akademischer Oberrat, Univ. Würzburg
2007–13	Elected member Users Org. Comm. (UOC), ESRF, Grenoble, France
Since 2008	Group Leader, Peter Grünberg Institute (PGI-3), FZ Jülich
Since 2012	Professor (W2) for Experimental Physics, RWTH Aachen
Since 2013	Member (since 2015 chair) of Peer Review Panel, Diamond Light Source, UK

Dr. Gerson Mette

Philipps-Universität Marburg, Department of Physics

gerson.mette@physik.uni-marburg.de PI since 07/2017

Expertise: Experimental physics, scanning probe microscopy, electron spectroscopy, non-linear laser spectroscopy of surfaces and interfaces, adsorption on metal and semiconductor surfaces

University Education

2007	Diploma degree in Physics (Dipl. Phys.), Univ. Marburg
2012	Doctoral degree in Physics (Dr. rer. nat.), Univ. Marburg

Professional Experience

2007–12	Research Assistant, Dept. of Physics, Univ. Marburg
2012–13	Res. secretary planned CRC 1083 and postdoc, Dept. of Physics, Univ. Marburg
2013	Marie-Curie Fellowship (European Commission)
2013–15	Postdoc, Dept. of Physics, Univ. Zürich, Switzerland
Since 2015	Research Associate, Dept. of Physics, Univ. Marburg

Prof. Dr. Michael Rohlfing

Westfälische Wilhelms-Universität Münster, Department of Physics

Michael.Rohlfing@wwu.de PI since 07/2017

Expertise: Theoretical physics, electronic-structure theory, many-body perturbation theory, excited electronic states, adsorbate systems, low-dimensional solids

University Education

1993	Diploma degree in Physics (Dipl. Phys.), WWU Münster
1996	Doctoral degree in Physics (Dr. rer. nat.), WWU Münster
2001	Habilitation in Theoretical Physics, WWU Münster

Professional Experience

1993–96	Research Assistant, WWU Münster
1997–98	Postdoc, Univ. of California at Berkeley, CA/USA
1999	Habilitation fellowship of the Deutsche Forschungsgemeinschaft
1999–03	Postdoc, WWU Münster
2001	Heisenberg fellowship of the Deutsche Forschungsgemeinschaft
2003–05	Assoc. Professor of Physics, Int. University (now: Jacobs University) Bremen
2005–13	Professor (W3) for Theoretical Physics, Univ. Osnabrück
Since 2013	Professor (W3) for Theoretical Physics, WWU Münster
Since 2013	Member computing-time advisory board, John-v-Neumann Inst. f. Computing Jülich

Dr. Daniel Sánchez-Portal

Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain

sqbsapod@ehu.es PI 10/2013-06/2017

Expertise: Theoretical condensed matter physics, electronic properties of surfaces and nano-structures, first-principles calculations, method and code development for electronic structure calculations

University Education

1993	Bachelor in Physics (B.Sc.), Univ. Autónoma Madrid, Spain
1989	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Frankfurt

Professional Experience

1993–99	Teaching Assistant, Univ. Autónoma Madrid, Spain
1999–00	Postdoc, Univ. of Illinois, Urbana, ILL/USA
2001	Postdoc, Univ. del País Vasco, San Sebastián, Spain
2002–05	Research Associate, "Ramón y Cajal"-program, CSIC-UPV/EHU, Spain
2005–08	Tenured Research Scientist, Centro de Física de Materiales, CSIC-UPV/EHU, Spain
Since 2008	Senior Research Scientist, Centro de Física de Materiales, CSIC-UPV/EHU, Spain
Since 2008	Member of the Barcelona Supercomputing Center Access Committee
2015	Elected Fellow of the American Physical Society (APS)

Dr. Martin Schmid

Philipps-Universität Marburg, Department of Chemistry

schmidm5@staff.uni-marburg.de PI 07/2017-09/2018

Expertise: Surface chemistry, model catalysis, organic and organometallic thin films, surface coordination chemistry, photoelectron spectroscopy, scanning tunneling microscopy

University Education

2008	Diplom degree in Physics (Dipl.-Phys.), Univ. Heidelberg
2012	Doctoral degree (Dr. rer. nat.), Univ. Erlangen-Nürnberg

Professional Experience

2012	Feodor-Lynen Fellowship of the Alexander von Humboldt Foundation
2012–14	Postdoc, Dept. of Chemistry and Chem. Biology, Harvard University
2014	Feodor-Lynen Return Fellowship of the Alexander von Humboldt Foundation
2014–18	Research Associate, Dept. of Chemistry, Univ. Marburg
2015	Liebig Fellowship of the Stiftung Stip.-Fonds d. Verb. d. Chem. Industrie e.V.

Prof. Dr. Wolfgang Stolz

Philipps-Universität Marburg, Dept. of Physics, Materials Science Center (WZMW)

wolfgang.stolz@physik.uni-marburg.de PI since 10/2013

Expertise: Epitaxial growth of III/V compound semiconductor heterostructures, structural, electrical and optoelectronic properties, optoelectronic device applications

University Education

1982	Diploma degree in Physics (Dipl. Phys.), Univ. Heidelberg & MPI Nuclear Physics
1986	Doctoral degree (Dr. rer. nat.), MPI Solid State Research & Univ. Stuttgart
1994	Habilitation in Experimental Physics, Univ. Marburg

Professional Experience

1995	Karl-Heinz-Beckurts-Prize (for Technology Transfer), Fed. Min. of Research & Technol.
Since 1999	Independent technology consultant
2002–09	Speaker of a DFG-Topical Research Group
2003	Prize of the German Society of Crystal Growth (DGKK)
2004	Co-founder and CTO of NAsP III/V GmbH, Marburg
Since 2007	Adjunct Professor, Optical Sciences Center, Univ. Arizona, Tucson, AZ/USA
2007–12	Coordinator of a BMBF-Joint Research Program
Since 2017	Professor (W3) for Exp. Physics, Semiconductor Physics, and Epitaxy, Univ. Marburg

Prof. Dr. Jörg Sundermeyer

Philipps-Universität Marburg, Department of Chemistry

jsu@staff.uni-marburg.de PI 10/2013-06/2017

Expertise: Inorganic molecule chemistry, coordination chemistry, organometallic chemistry, homogeneous catalysis, biphase catalysis, functional molecules for material chemistry

University Education

1984	Diploma degree in Chemistry (Dipl. Chem.), Univ. Göttingen
1988	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Göttingen
1995	Habilitation in Inorganic Chemistry, Univ. Würzburg

Professional Experience

1984–85	Research Assistant, C.S.I.R. Unit of Metal Cluster Chemistry, Rep. of South Africa
1986–88	Research Assistant, Univ. Göttingen
1989–91	Liebig-Stipend of the Stiftung Stip.-Fonds d. Verb. d. Chem. Industrie e.V.
1989–95	Research Associate, Univ. Würzburg
1991–93	Habilitation-Stipend of the German Research Foundation (DFG)
1994	Heinz-Maier-Leibnitz-Award, Federal Ministry for Education and Science
1995–96	Lecturer, Univ. Würzburg
1996	Heisenberg-Fellow of the German Research Foundation (DFG)
Since 1996	Professor for Organometallic Chemistry, Univ. Marburg

Prof. Dr. Frank Stefan Tautz

Forschungszentrum Jülich (FZ Jülich), Peter Grünberg Institut (PGI-3)

s.tautz@fz-juelich.de PI since 07/2017

Expertise: Surface and interface science, electron and X-ray diffraction, photoelectron microscopy and tomography, low temp. scanning probe microscopy

University Education

1990	MPhil in Theoretical Physics, Univ. of Cambridge, UK
1994	PhD in Experimental Physics, Univ. of Cambridge, UK
2001	Habilitation in Experimental Physics, TU Ilmenau

Professional Experience

1989–1990	Study-abroad scholarship, Dr. Carl Duisberg Gesellschaft
1990–91	Scholarship, Deutscher Akademischer Austauschdienst (DAAD)
1991–93	Scholarship, James-Clerk-Maxwell Studentship in Experimental Physics
1993	Scholarship, Cambridge Philosophical Society
1994–95	Postdoc, van der Waals-Zeeman Lab., Univ. Amsterdam, Netherlands
1995–01	Research Assistant (C1), TU Ilmenau
2001	Research Assistant (C2), TU Ilmenau
2001–07	Associate Professor of Physics, Int. Univ.Bremen (now: Jacobs Univ. Bremen)
Since 2007	W3 Professor, RWTH Aachen
Since 2007	Director, Peter Grünberg Inst. (PGI-3), Forschungszentrum Jülich
2016	Invited core member of long program at Inst. of Pure and Applied Mathematics, UCLA, CA/USA

PD Dr. Ralf Tonner

Philipps-Universität Marburg, Department of Chemistry

tonner@chemie.uni-marburg.de PI since 10/2013

Expertise: Computational chemistry, density functional theory, surface chemistry, inorganic chemistry, chemical bonding, molecular crystals

University Education

2003	Diploma degree in Chemistry (Dipl. Chem.), Univ. Marburg
2007	Doctoral degree in Chemistry (Dr. rer. nat.), Univ. Marburg
2016	Habilitation in Theoretical Chemistry, Univ. Marburg

Professional Experience

2004–07	Research Assistant, Chem. Department, Univ. Marburg
2008	Postdoctoral Fellowship of the DAAD (1 yr)
2008–10	Postdoc, Centre f. Theoret. Chem. & Physics, Massey Univ., Auckland, NZL
2009	Feodor Lynen-Fellowship of the Alexander von Humboldt Foundation (2 yrs)
2010-19	Jun. Res. Group Leader Theoretical Surface Chemistry, Univ. Marburg
2015	Visiting Ass. Professor, Dept. of Chem. Eng., Stanford Univ., CA/USA
2016	"Hans G. A. Hellmann Prize for Theoretical Chemistry" of the AGTC

Prof. Dr. Kerstin Volz

Philipps-Universität Marburg, Dept. of Physics, Materials Science Center (WZMW)

kerstin.volz@physik.uni-marburg.de PI since 10/2013

Expertise: Experimental physics, transmission electron microscopy, epitaxial growth of semiconductors, correlation of structural characteristics in functional materials

University Education

1996	Diploma degree in Physics (Dipl. Phys.), Univ. Augsburg
1999	Doct. degr. in Phys.(Dr. rer. nat.), Univ. Augsburg / GSI Darmstadt / Univ. Marburg
2006	Habilitation in Experimental Physics, Univ. Marburg

Professional Experience

1997–00	Several research stays at Osaka National Research Laboratory, Japan
2001–02	Feodor Lynen Scholarship of A. von Humboldt Stiftung, Stanford Univ., CA/USA
2003–08	DFG-Junior Research Group Leader, WZMW, Univ. Marburg
Since 2009	Heisenberg-Professor of DFG for Experimental Physics, Univ. Marburg
Since 2010	"Internetportal für exz. Wissenschaftlerinnen", Robert-Bosch Foundation & Spektrum-Verlag
Since 2012	Speaker of Research Training Group GRK 1782, Univ. Marburg
Since 2013	Vice Speaker of Collaborative Research Center SFB 1083, Univ. Marburg
Since 2015	Managing director of the WZMW
Since 2016	Member of the MRS Wedal Selection Committee
Since 2018	Member of the Managing Board of the German Society for Electron Microscopy (DGE)
Since 2018	Dean of the Department of Physics, Univ. Marburg

Dr. Robert Wallauer

Philipps-Universität Marburg, Department of Physics

robert.wallauer@physik.uni-marburg.de PI since 07/2017

Expertise: Experimental physics, strongly correlated electron systems, electron spectrometers, laser- and synchrotron-based photoelectron spectroscopy

University Education

2006	Diploma degree in Physics (Dipl. Phys.), Univ. Frankfurt
2012	Doctoral degree in Physics (Dr. phil. nat.), Univ. Frankfurt

Professional Experience

2005–06	Research stay Inst. Pluridisciplinar, Complutense University, Madrid, Spain
2013	Minerva Fellowship (Max Planck Society)
2006–13	Research Assistant, Institute of Nuclear Physics (Prof. R. Dörner), Univ. Frankfurt
2013–14	Postdoc, Faculty of Physics, Technion – Israel Institute of Technology, Haifa, Israel
2015–16	Postdoc, Institute of Physics, Univ. Mainz
Since 2016	Research Accociate, Dept. of Physics, Univ. Marburg

Dr. Christof Wegscheid-Gerlach

Philipps-Universität Marburg, Department of Pharmacy

wegscheid-gerlach@staff.uni-marburg.de PI since 07/2017

Expertise: Pharmaceutical chemistry, computer aided molecular design, molecular modelling, pharmaceutical and chemical education

University Education

2002	State licensed pharmacist
2006	Doctoral degree in Pharmaceutical Chemistry (Dr. rer. nat.), Univ. Marburg

Professional Experience

2001–02	Practical training for pharmacists, Hoffmann La-Roche, Basel
2002	Practical training for pharmacists, Apotheke am Brommygrün, Wilhelmshaven
2003–06	Stipend of a DFG-research training group
2006–07	Postdoc in computational chemistry, Lilly Pharma, Hamburg
2007–08	Assoc. member of an EU FP7 Marie Curie Res. Training Network
2007–09	Lab Head computational chemistry, Bayer Health Care, Berlin
2010–13	Permanent position as staff scientist, Univ. Marburg
Since 2011	Deputy Executive Director Chemikum Marburg e.V.
Since 2013	Permanent position as “Akademischer Rat”, Univ. Marburg
Since 2014	Member of the academic senate at Philipps-Universität Marburg

Prof. Dr. Gregor Witte

Philipps-Universität Marburg, Department of Physics

gregor.witte@physik.uni-marburg.de PI since 10/2013

Expertise: Organic semiconductor films, physical chemistry of adsorbates, template and interface controlled growth of thin films, X-ray absorption spectroscopy

University Education

1989	Diploma degree in Physics (Dipl. Phys.), Univ. Göttingen
1995	Doctoral degree in Physics (Dr. rer. nat.), Univ. Göttingen
2002	Habilitation in Physical Chemistry, Univ. Bochum

Professional Experience

1989–90	Research Assistant, MPI for Dynamics and Self-Organization, Göttingen
1990–91	“ORFEUS” project assistant: optical alignment of space shuttle based UV-telescope, München
1991–95	Research Assistant, MPI for Strömungsforschung, Göttingen
1996	Postdoctoral Fellowship of the DFG
1996–97	Postdoc, IBM Res. Ctr, San Jose & Lawrence Berkeley Nat. Lab., Berkeley, CA/USA
1998–02	Group Leader (Research Assistant), Univ. Bochum
2003–08	Lecturer (Dozent) (C2), Dept. of Chemistry, Univ. Bochum
Since 2008	Professor (W3) for Experimental Physics, Univ. Marburg

Research Network

Prof. Dr. James Hone
Department of Mechanical Engineering, Columbia University, New York, USA

Prof. Dr. David Johnson
Center for Sustainable Materials Chemistry
University of Oregon, Corvallis, USA

Prof. Dr. Hrvoje Petek
Department of Physics and Astronomy
University of Pittsburgh, USA

Prof. Dr. Christopher Stanton
Department of Physics
University of Florida, Gainesville, USA

Prof. Dr. Mackillo Kira
Department of Electrical Engineering
University of Michigan, Ann Arbor, MI/USA

Dr. Kunie Ishioka
National Institute for Materials Science (NIMS)
Tsukuba, Japan

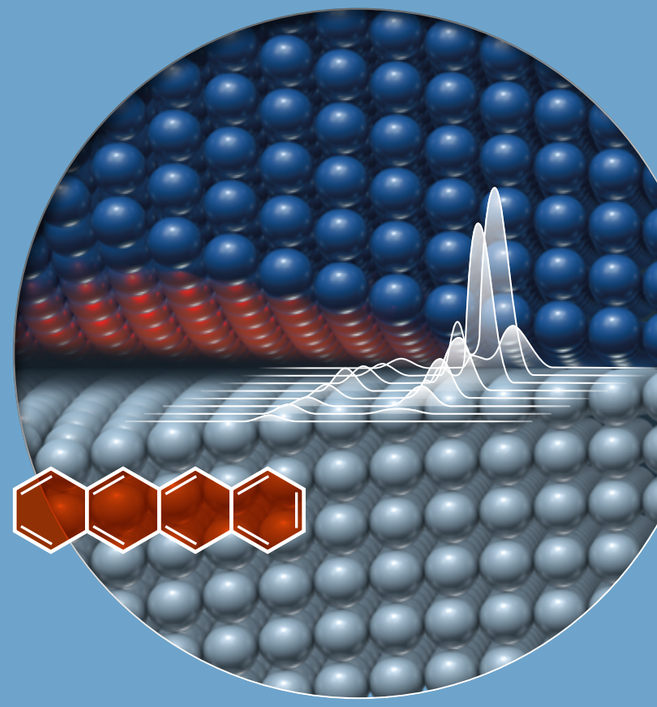
Prof. Dr. Pedro M. Echenique
Donostia International Physics Center (DIPC)
San Sebastián, Spain

Dr. Daniel Sánchez-Portal
Centro de Fisica de Materiales, CSIC-UPV/EHU und DIPC
San Sebastián, Spain

SFB 1083 was established in 2013 as a classical Sonderforschungsbereich, located solely at the Philipps-Universität Marburg. For its 2nd funding period, two groups of Justus-Liebig-Univesität Gießen, one of Forschungszentrum Jülich and one of Westfälische Wilhelms-Universtität in Münster were invited to join the Center. They strengthen the scientific programme with complementary expertise in the field of internal interfaces.

Research of SFB 1083 benefits from a strong network of international collaborations. A guest project at one of the worldwide leading institutions for solid-state theory, the Donostia International Physics Center (DIPC) in San Sebastián, Spain, strongly contributed to the scientific programme of the 1st funding period. Moreover, two US groups in Pittsburgh and Gainesville/Florida were associated via the Materials World Network, jointly funded by the German DFG and the American NSF. As of today, SFB 2083 comprises a total of eight associated members in Europe, the United States and Japan.

VISITORS



Guest Scientists

2013

Dr. Osmo Vänskä, Aalto University, Finland
18.11.–29.11.2013, Project B4 (SW Koch/Kira)
charge-transfer excitons in type-II semiconductor heterostructures

Prof. Dr. Christopher J. Stanton, University of Florida, Gainesville, USA
25.11.–30.11.2013, Project B5 (Höfer)
optical and acoustic phonons at GaP/Si interfaces

Prof. Dr. Hrvoje Petek (external member), University of Pittsburgh, USA
26.11.–01.12.2013, Project B5 (Höfer)
electron-lattice dynamics at atomic-controlled interfaces

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
26.11.–04.12.2013, Project B5 (Höfer)
coherent phonon spectroscopy of semiconductors interfaces

Dr. Nikolay Zaitsev, National Research Tomsk State University, Russia
27.11.–12.12.2013, Project A6 (Tonner) & GP1 (Echenique/Sanchez)
DFT calculations of metal/organic interfaces

2014

Dr. Kenta Kuroda (JSPS Overseas Fellow), Hiroshima University, Japan
01.04.2014–07.05.2015, Project B6 (Höfer)
surface photocurrents of topological insulators

Prof. Dr. Hrvoje Petek (A. v. Humboldt Award), University of Pittsburgh, USA
15.05.–29.05.2014, Project B5 (Höfer)
electron-lattice dynamics at atomic-controlled interfaces

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
22.05.–29.05.2014, Project B5 (Höfer)
coherent phonon spectroscopy of semiconductors interfaces

Prof. Dr. Toshiaki Munakata, Osaka University, Japan
11.06.–02.08.2014, Project B6 (Höfer)
two-photon photoemission spectroscopy of organic interfaces

Dr. Henning Döscher (Marie-Curie Fellow), National Renewable Energy Laboratory, Colorado, USA
01.08.2014–30.09.2015, Project A1 (Stolz)
reflection anisotropy spectroscopy of epitaxial semiconductor growth

Dr. Frederik M. Schiller (Fellow, CSIC Spain), Centro de Física de Materiales, San Sebastián, Spain
15.09.2014–10.08.2016, Project B6 (Höfer)
electron transfer at molecule-metal junctions

Prof. Dr. Hrvoje Petek (A. v. Humboldt Award), University of Pittsburgh, USA
16.11.–01.12.2014, Project B5 (Höfer)
electron-lattice dynamics at atomic-controlled interfaces

2015

Dr. Kenta Kuroda (JSPS Overseas Fellow), Hiroshima University, Japan
01.04.2014–07.05.2015, Project B6 (Höfer)
surface photocurrents of topological insulators

Dr. Henning Döscher (Marie-Curie Fellow), National Renewable Energy Laboratory, Colorado, USA
01.08.2014–30.09.2015, Project A1 (Stolz)
reflection anisotropy spectroscopy of epitaxial semiconductor growth

Dr. Frederik M. Schiller (Fellow, CSIC Spain), Centro de Física de Materiales, San Sebastián, Spain
15.09.2014–10.08.2016, Project B6 (Höfer)
electron transfer at molecule-metal junctions

Prof. Dr. Stacey Bent, Stanford University, USA
27.04.–02.05.2015, Project A6 (Tonner) & B5 (Höfer)
molecular functionalization of semiconductor surfaces

Prof. Dr. Talat S. Rahman, University of Central Florida, Orlando, USA
28.04.–01.05.2015, Project A2 (Witte)
modeling chemical reactions and phenomena at surfaces

Dr. Juan Pablo Echeverry Enciso, Humboldt Universität zu Berlin
30.04.–01.07.2015, Project A2 (Witte)
theoretical description of optical excitations in pentacene molecular crystals

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
02.08.–12.08.2015, Project B5 (Höfer)
coherent phonon spectroscopy of semiconductor interfaces

Prof. Dr. Talat S. Rahman, University of Central Florida, Orlando, USA
07.11.–16.11.2015, Project A2 (Witte)
modeling chemical reactions and phenomena at surfaces

2016

Dr. Frederik M. Schiller (Fellow, CSIC Spain), Centro de Física de Materiales, San Sebastián, Spain
15.09.2014–10.08.2016, Project B6 (Höfer)
electron transfer at molecule-metal junctions

Dr. Kenta Kuroda, University of Tokyo, Japan
03.03.–11.03.2016, Project B6 (Höfer)
surface photocurrents of topological insulators

Dr. Leander Tapfer, ENEA Centro Ricerche, Brindisi, Italy
02.05.–14.05.2016, Project A1 (Stolz)
high resolution x-ray diffraction in GaP_xAs_{1-x}-films

Prof. Dr. Toshiaki Munakata, Osaka University, Japan
29.05.–05.06.2016, Project B6 (Höfer)
two-photon photoemission spectroscopy of organic interfaces

Prof. Dr. Yoshiyasu Matsumoto, Kyoto University, Japan
30.05.–05.06.2016, Project B6 (Höfer)
interfaces of ice crystal films

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
30.05.–08.06.2016, Project B5 (Höfer)
coherent phonon spectroscopy of semiconductor interfaces

Prof. Dr. Hrvoje Petek (external member), University of Pittsburgh, USA
30.05.–03.06.2016, Project B5 (Höfer)
electron-lattice dynamics at atomic-controlled interfaces

Prof. Dr. Christopher J. Stanton (external member), University of Florida, Gainesville, USA
30.05.–03.06.2016, Project B5 (Höfer)
optical and acoustic phonons at GaP/Si interfaces

Prof. Dr. David C. Johnson, University of Oregon, Eugene, USA
21.10.–25.10.2016, Project A9 (Dehnen)
synthesis of dichalcogenides multilayer stacks

Dr. Jorge Lobo Checa, Universidad de Zaragoza, Spain
01.12.–14.12.2016, Project B6 (Höfer)
image-potential states of porous molecular networks

Dr. Frederik M. Schiller, Centro de Física de Materiales, San Sebastián, Spain
06.12.–15.12.2016, Project B6 (Höfer)
image-potential states of porous molecular networks

2017

Dr. Qitang Fan (A. v. Humboldt Fellow), University of Science and Technology, Hefei, China
01.01.2017–31.12.2018, Project A4 (Gottfried)
surface-assisted organic synthesis

Prof. Dr. John F. Corrigan, Western University, London, Canada
19.02.–19.03.2017, Project A9 (Dehnen)
synthesis and structural characterization of metal chalcogenide clusters and nanoparticles

Prof. Dr. Hrvoje Petek (external member), University of Pittsburgh, USA
03.03.–08.03.2017, Project B5 (Höfer)
electron-lattice dynamics at atomic-controlled interfaces

Prof. Dr. Maki Kawai (A. v. Humboldt Award), University of Tokyo, Japan
28.04.–03.05.2017, Projekt A4 (Gottfried) & B5 (Höfer)
chemical reactions at interfaces

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
20.08.–22.08.2017, Project B5 (Höfer/Mette)
coherent phonon spectroscopy of semiconductor interfaces

Dr. Kento Uchida, Kyoto University, Japan
01.10.–27.11.2017, Project B3 (M Koch/Heimbrodt)
strong THz radiation spectroscopy

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
08.10.–15.10.2017, Project B5 (Höfer/Mette)
coherent phonon spectroscopy of semiconductor interfaces

2018

Dr. Qitang Fan (A. v. Humboldt Fellow), University of Science and Technology, Hefei, China
01.01.2017–31.12.2018, Project A4 (Gottfried)
surface-assisted organic synthesis

Prof. Dr. Ewan Wright, University of Arizona, Tucson, USA
01.06.–30.06.2018, Project B4 (SW Koch) & B5 (Höfer/Mette)
non-linear optical effects in condensed matter systems

Prof. Dr. Junfa Zhu, University of Science and Technology of China, Hefei, China
06.07.–09.07.2018, Project A4 (Gottfried)
transition metal-organic interfaces

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
10.07.–14.07.2018, Project B5 (Höfer/Mette)
coherent phonon spectroscopy of semiconductor interfaces

Prof. Dr. Akio Kimura, Hiroshima University, Japan
19.07.–21.07.2018, Project B6 (Höfer/Wallauer)
time-resolved two-photon photoemission of doped topological insulators

Prof. Dr. Daniel M. Mittleman (A. v. Humboldt Award), Brown University, Providence, USA
12.08.–18.08.2018, Project B3 (M Koch/Heimbrodt)
spectroscopy and imaging with THz radiation

Dr. Kazuki Sumida, Hiroshima University, Japan
01.10.–19.10.2018, Project B6 (Höfer/Wallauer)
time-resolved two-photon photoemission of doped topological insulators

Prof. Dr. Akio Kimura, Hiroshima University, Japan
16.10.–20.10.2018, Project B6 (Höfer/Wallauer)
time-resolved two-photon photoemission of doped topological insulators

Prof. Dr. Eyad Younes, Hashemite University, Jordan
13.11.–15.11.2018, Project A8 (Koert/Dürr)
organic and materials chemistry

2019

Dr. Arslan Usman (A. v. Humboldt Fellow), COMSATS University Islamabad, Pakistan
01.02.2019–01.02.2021, Project B3 (M Koch/Heimbrodt)
optical spectroscopy on 2D materials

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
03.02.–14.02.2019, Project B5 (Höfer/Mette)
coherent phonon spectroscopy of semiconductor interfaces

Dr. Suguru Ito (JSPS Overseas Fellow), University of Tokyo, Japan
11.04.2019–10.04.2021, Project B5 (Höfer/Mette)
THz-excited time-resolved photoelectron spectroscopy

Prof. Dr. Katsumi Tanimura, Osaka University, Japan
12.05.–18.05.2019, Project B6 (Höfer/Mette)
time-resolved photoemission of TMDC interfaces

Prof. Dr. Yoshihiro Miyauchi, National Defense Academy, Kanagawa, Japan
13.05.–17.05.2019, Project B5 (Höfer/Mette)
microscopy of optical generation of second harmonics

Prof. Dr. Daniel M. Mittleman (A. v. Humboldt Award), Brown University, Providence, USA
01.06.–31.07.2019, Project B3 (M Koch/Heimbrodt)
spectroscopy and imaging with THz radiation

Dr. Hilary Masenda (A. v. Humboldt Fellow), University of the Witwatersrand, Johannesburg, South Africa
01.06.2019–31.05.2021, Project B3 (M Koch/Heimbrodt)
2D materials and van der Waals heterostructures

Prof. Dr. Hiroyuki Yoshida, Chiba University, Japan
11.06.–18.06.2019, Project A12 (Tautz/Bocquet/Kumpf)
high-resolution inverse photoemission spectroscopy for quantum computing-relevant interfaces

Prof. Dr. Jerome Moloney, University of Arizona, Tucson, USA
16.06.–18.06.2019, Project B7 (Stolz/SW Koch)
type-II W-quantum well lasers

Dr. Kunie Ishioka (external member), National Institute for Materials Science, Tsukuba, Japan
15.09.–18.09.2019, Project B5 (Höfer/Mette)
coherent phonon spectroscopy of semiconductor interfaces

Prof. Dr. Katsumi Tanimura, Osaka University, Japan
15.08.–02.11.2019, Project B6 (Höfer/Wallauer)
time-resolved photoemission of TMDC interfaces

Prof. Dr. Kyoko Ishizaka, University of Tokyo, Japan
15.12–20.12.2019, Project A5 (Volz) & B5 (Höfer/Mette)
time-resolved TEM of strain waves in GaP/Si(001)

Dr. Takahiro Shimojima, Riken, Saitama, Japan
15.12–20.12.2019, Project A5 (Volz) & B5 (Höfer/Mette)
time-resolved TEM of strain waves in GaP/Si(001)

Short Term Visitors, Colloquia and Lectures

2013

Prof. Dr. Torsten Fritz, Friedrich-Schiller-Universität Jena (31.10.2013)
"Optical in situ differential reflectance spectroscopy on epitaxially grown molecular films"

Prof. Dr. Katsumi Tanimura, Osaka University, Japan (01.11.2013)
"Time-resolved photoemission study of ultrafast carrier dynamics in GaAs and InP"

Prof. Dr. Petra Tegeder, Universität Heidelberg (14.11.2013)
"Electronic properties of interfaces with organic compounds"

Dr. Kunie Ishioka, National Institute for Materials Science, Tsukuba, Japan (27.11.2013)
Kick-off Meeting: "Coherent phonons at the GaP/Si interface"

Dr. Peter Koval, Donostia International Physics Center, San Sebastián, Spain (27.11.–29.11.2013)
Kick-off Meeting: "Using basis sets of local functions for efficient TDDFT and GW calculations"

Dr. Gerson Mette, Universität Zürich, Switzerland (27.11.–29.11.2013)
Kick-off Meeting: "Adsorption of cyclooctyne on Si(100)"

Dr. Ilya Nechaev, Donostia International Physics Center, San Sebastián, Spain / Tomsk State University, Russia (27.11.–29.11.2013)
Kick-off Meeting: "DFT investigation of organic/metal interface states"

Prof. Dr. Moritz Sokolowski, Universität Bonn (12.12.2013)
"Fluorescence spectroscopy and of large organic molecules on surfaces"

Prof. Dr. Thorsten Fritz, Friedrich-Schiller-Universität Jena (17.12.2013)
"Optical in situ differential reflectance spectroscopy on epitaxially grown molecular films"

2014

Dr. Tobias Kampfrath, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (30.01.2014)
"Beyond body scanners: how to use terahertz pulses to observe and control spin dynamics in solids"

Dr. Mathias Ljungberg, Université de Bordeaux, Talence, France (28.03.2014)
"Efficient solution of the GW and Bethe-Salpeter equation methods in a local basis"

Dr. Kenta Kuroda, Hiroshima University, Japan (11.04.2014)
"Bulk carrier manipulation of ideal topological insulator $TlBiSe_2$ in reversible spin current regime"

Dr. Christian Udhardt, Friedrich-Schiller-Universität Jena (25.04.2014)
"Resonant excitation at the rubrene/graphite interface"

Dr. Christian Schwalb, Philipps-Universität Marburg (30.04.2014)
"A novel sensing method for atomic force microscopy using nanogranular metals"

Prof. Dr. Christof Wöll, Karlsruher Institut für Technologie (15.05.2014)
"From the molecule to the functional material: quasi epitaxial growth of metal-organic frameworks (MOFs) on modified substrates"

Prof. Dr. Hrvoje Petek, University of Pittsburgh, USA (20.05.2014)
"Atomic scale imaging of CO_2 capture by metal-organic frameworks"

Prof. Dr. Juan José Sáenz, Universidad Autónoma de Madrid, Spain (12.06.2014)
"Scattering asymmetry and non-conservative optical forces"

Prof. Dr. Toshiaki Munakata, Osaka University, Japan (13.06.2014)
"Electronic excitation in rubrene"

Dr. Laura Fernandez, Centro de Física de Materiales, San Sebastián, Spain (23.06.2014)
"Co nanodot arrays grown on $REAu_2$ nanotemplates: substrate/nanodot magnetic coupling"

Prof. Dr. Kazuyuki Sakamoto, Chiba University, Japan (24.06.2014)
"Peculiar Rashba spins on silicon surfaces"

Prof. Dr. Philip P. Power, University of California, Davis, USA (25.06.2014)
"Low, 2- or 3-coordinate transition metal complexes and their magnetic properties"

Prof. Dr. Robert Berger, TU Darmstadt (03.07.2014)
"Quantum chemistry for the interface"

Dr. Frederik Schiller, Centro Física de Materiales, San Sebastián, Spain (04.07.2014)
"The effect of nanostructuring on electronic properties of metals"

Dr. Frederic Laquai, Max-Planck-Institut für Polymerforschung, Mainz (17.07.2014)
"The role of charge transfer excitons in photorecurrent generation in excitonic solar cells"

Prof. Dr. Satoshi Kera, Institute for Molecular Science, Okazaki, Japan (17.07.2014)
"Violation of sudden approximation at molecular monolayer interface"

Prof. Dr. Toshiaki Munakata, Osaka University, Japan (17.07.2014)
"Unoccupied states of organic films observes by 2PPE and STM"

Prof. Dr. Stefan Tautz, Peter Grünberg Institut, FZ Jülich (17.07.2014)
"Towards an atomistic understanding of molecule-metal-interfaces"

Dr. Andrés Arnau, Donostia International Physics Center, San Sebastián, Spain (28.07.–30.07.2014)
Summer School, San Sebastián: "Electronic properties of molecular overlayers on surfaces"
& "Electronic and magnetic properties of metal-organic coordination networks"

Prof. Dr. Michael Dürr, Justus-Liebig-Universität Gießen (28.07.–30.07.2014)
Summer School, San Sebastián: "Reactions of organic molecules on semiconductor surfaces –
part 1: mechanisms & part 2: towards controlled functionalization"

Prof. Dr. Tony Heinz, Columbia University in the City of New York, USA (28.07.–30.07.2014)
Summer School, San Sebastián: "Electronic and optical properties of atomically thin 2D materials"
& "Many-body effects in the optical response of atomically thin 2D materials"

Prof. Dr. Leeor Kronik, Weizmann Institute of Science, Israel (28.07.–30.07.2014)
Summer School, San Sebastián: "Understanding organic/inorganic interfaces from first principles"
& "Collective effects at organic/inorganic interfaces"

Prof. Dr. Thomas Kuech, University of Wisconsin-Madison, USA (28.07.–30.07.2014)
Summer School, San Sebastián: "Epitaxial formation of multilayer structures: the interplay of thermodynamics,
kinetics and growth behavior" & "The formation of metastable alloys"

Prof. Dr. Susanne Stemmer, University of California, Santa Barbara, USA (28.07.–30.07.2014)
Summer School, San Sebastián: "Quantitative scanning transmission electron microscopy" & "Complex oxide interfaces"

Prof. Dr. Wilfried Wurth, Deutsches Elektronen-Synchrotron, Universität Hamburg (28.07.–30.07.2014)
Summer School, San Sebastián: "X-ray spectroscopy – a great toolbox for the study of interfaces"
& "Time-resolved X-ray spectroscopy at free-electron laser sources"

Prof. Dr. Xiaoyang Zhu, Columbia University in the City of New York, USA (28.07.–30.07.2014)
Summer School, San Sebastián: "Excitons at organic semiconductor interfaces" & "Exciton fission and solar energy
conversion beyond the limit"

Dr. Ilya Nechaev, Donostia International Physics Center, San Sebastián, Spain (20.11.2014)
"Lifetimes of interface and image-potential states in metal-organic interfaces as estimated within one-dimensional
pseudopotential model"

Prof. Dr. Enrique Ortega, Universidad del País Vasco, San Sebastián, Spain (27.11.2014)
"Electronic states at donor/acceptor metal interfaces probed with electron spectroscopies"

Prof. Dr. Frank Würthner, Julius-Maximilians-Universität Würzburg (18.12.2014)
"Dye assemblies for supramolecular electronics & photovoltaics"

2015

Prof. Dr. Hans-Peter Steinrück, Friedrich-Alexander Universität Erlangen-Nürnberg (15.01.2015)
"Surface Science of Complex Molecular Systems"

Dr. Koji Miyamoto, Westfälische Wilhelms-Universität Münster (19.01.2015)
"Spin polarization of Dirac-cone-like surface state at W(110) – orbital-selective spin characterization
& lightpolarization-induced spin effect"

Prof. Dr. Claudia Draxl, Humboldt-Universität zu Berlin (29.01.2015)
"Theoretical spectroscopy of molecules and their condensed phases"

Dr. Konrad Gillmeister, Martin-Luther-Universität Halle-Wittenberg (30.01.2015)
"The ultrashort life of excited electrons in NiO"

Dr. Ian Howard, Karlsruher Institut für Technologie (04.02.2015)
"The role of charge-transfer excitons in determining the efficiency of organic solar cells"

Prof. Dr. Michael Horn-von Hoegen, Universität Duisburg-Essen (01.03.–06.03.2015)
WUPCOM'15, Winklmoosalm: "Electron Diffraction at Surfaces: by now Ultrafast!"

Prof. Dr. Holger Bettinger, Eberhard Karls Universität Tübingen (16.04.2015)
"Graphene substructures without and with Boron-Nitrogen-substitution"

Dr. Christoph Heyl, Lund University, Sweden (27.04.2015)
"Status and prospects of high repetition rate high-order harmonic and attosecond sources"

Prof. Dr. Maki Kawai, University of Tokyo, Japan (27.04.2015)
"Chemistry and electron dynamics of molecules at surfaces"

Prof. Dr. Stacey Bent, Stanford University, USA (28.04.2015)
"Molecular functionalization of semiconductor surfaces"

Prof. Dr. Talat Rahman, University of Central Florida, Orlando, USA (29.04.2015)
"Tailoring properties of single layer MoS_2: looking beyond graphene"

Prof. Dr. Rudolf Bratschitsch, Westfälische Wilhelms-Universität Münster (30.04.2015)
"Atomically thin transition metal dichaocogenides light up"

Prof. Dr. Jörg Neugebauer, Max-Planck-Institut für Eisenforschung, Düsseldorf (07.05.2015)
"Ab initio thermodynamics: a novel route to design materials on the computer"

Dr. Shekhar Priyadarshi, Physikalisch-Technische Bundesanstalt Braunschweig (12.05.2015)
"Coherent control of all-optically induced currents with polarization shaped optical pulses"

Dr. Alexander V. Chernenko, Russian Academy of Sciences, Chernogolovka, Russia (19.05.2015)
"Localized and bound excitons in type-II ZnMnSn/ZnSSe quantum wells"

Prof. Dr. Huizhen Wu, Zhejiang University, China (11.06.2015)
"2DEG at the interface od CdTe(zincblende)/PbTe(rock-salt) heterostructures"

Prof. Dr. Thomas Chassé, Eberhard Karls Universität Tübingen (25.06.2015)
"Organic films for electronics and optoelectronics – reactions, interfaces"

Prof. Dr. Frank Schreiber, Eberhard Karls Universität Tübingen (09.07.2015)
"Charge transfer effects at interfaces"

Prof. Dr. Julia Stähler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (03.08.–06.08.2015)
"Exciting! What happens when light is absorbed in a semiconductor?"

Dr. Kunie Ishioka, National Institute for Materials Science, Tsukuba, Japan (05.08.2015)
"Ultrafast spectroscopy for materials science"

Prof. Dr. Akio Kimura, Hiroshima University, Japan (04.09.2015)
"Surface Dirac fermion dynamics and spin polarizations of three-dimensional topological insulators"

Prof. Dr. Kazuya Watanabe, Kyoto University, Japan (07.09.2015)
"Ultrafast vibrational dynamics at metal surfaces"

Dr. Reza Kakavandi, Eberhard-Karls-Universität Tübingen (14.09.2015)
"Highly controlled deposition of organic magnets on metal-oxide surfaces"

Dr. Jan Mertens, University of Cambridge, UK (05.10.2015)
"Plasmonics meets 2D materials: image-coupled sub-nanometre cavities"

Prof. Dr. Erwin Kessels, Eindhoven University of Technology, Netherlands (11.11.2015)
"Atomic layer deposition of Al2O3: new insights from sum-frequency generation studies"

PD Dr. Achim Schöll, Julius-Maximilians-Universität Würzburg (12.11.2015)
"Photoelectron spectroscopy of organic layers and interfaces: from orbital mapping to Kondo physics"

Prof. Dr. Michael G. Ramsey, Karl-Franzens Universität Graz, Austria (26.11.2015)
"Imaging the orbitals of adsorbed molecules with photoemission tomography"

Prof. Dr. Toshiaki Munakata, Osaka University, Japan (02.12.2015)
"Carrier dynamics of molecules by two-photon photoemission (2PPE) spectroscopy"

Prof. Dr. Alessandro Troisi, University of Warwick, UK (10.12.2015)
"Interesting electronics processes in organic semiconductors: from ultrafast to ultraslow"

Prof. Dr. Christian Kumpf, FZ Jülich and RWTH Aachen (17.12.2015)
"On geometric and electronic fingerprints of the molecule-substrate interaction at hetero-organic interfaces"

2016

Prof. Dr. Peter Saalfrank, Universität Potsdam (14.01.2016)
"Non-adiabatic dynamics at surfaces"

Dr. Ralph Ernstorfer, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (22.01.2016)
"Accessing electron-phonon interaction with time-resolved diffraction and XUV-based trARPES"

Dr. Alexander V. Chernenko, Russian Academy of Sciences, Chernogolovka, Russia (28.01.2016)
"Electronic structure and electron dynamics in novel two-dimensional materials"

Prof. Dr. Philip Hofmann, Aarhus University, Denmark (11.02.2016)
"Electronic structure and electron dynamics in novel two-dimensional materials"

Dr. Hagen Klauk, Max-Planck-Institut für Festkörperforschung, Stuttgart (28.01.2016)
"Low-voltage organic thin-film transistors for flexible displays"

Dr. Kenta Kuroda, University of Tokyo, Japan (04.03.2016)
"Ultrafast dynamics of photocurrents in the Dirac cone of the surface state of a topological insulator"

Prof. Dr. Josef Wachtveitl, Goethe-Universität Frankfurt am Main (14.04.2016)
"Ultrafast interfacial electron transfer in nanoscale systems"

Prof. Dr. Jochen Kuhn, TU Kaiserslautern (18.04.2016)
"Lernen in Schülerlaboren – Chancen und Grenzen öffentlicher Lernorte"

Prof. Dr. Rupert Huber, Universität Regensburg (28.04.2016)
"Faster than a cycle of light"

Dr. Martin Mittendorff, University of Maryland, USA (28.04.2016)
"THz properties of 2D semiconductors: time resolved spectroscopy and applications"

Dr. Alexander Hinderhofer, Eberhard Karls Universität Tübingen (12.05.2016)
"Structure and ionization energies of organic semiconductor thin film blends"

Dr. Shigeki Kawai, Universität Basel, Switzerland (20.05.2016)
"Mechanical and chemical properties of molecules studied by high-resolution atomic force microscopy"

Prof. Dr. Martin Aeschlimann, Universität Kaiserslautern (31.05.–03.06.2016)
ICII-2016, Marburg: "Controlling the spin texture of topological insulators with organic molecules"

Prof. Dr. Silvana Botti, Friedrich-Schiller-Universität Jena (31.05.–03.06.2016)
ICII-2016, Marburg: "Materials design at interfaces for photovoltaics"

Prof. Dr. Friedhelm Bechstedt, Friedrich-Schiller-Universität Jena (31.05.–03.06.2016)
ICII-2016, Marburg: "Topological states at semiconductor interfaces: a view from first principles"

Prof. Dr. Torsten Fritz, Friedrich-Schiller-Universität Jena (31.05.–03.06.2016)
ICII-2016, Marburg: "Epitaxy without coincidences – the stabilizing role of static distortion waves"

Prof. Dr. James Hone, Columbia University in the City of New York, USA (31.05.–03.06.2016)
ICII-2016, Marburg: "2D materials in the ultraclean limit: basic science and applications"

Prof. Dr. Norbert Koch, Humboldt-Universität zu Berlin (31.05.–03.06.2016)
ICII-2016, Marburg: "Energy level tuning at inorganic/organic semiconductor heterojunctions"

Prof. Dr. Steven Louie, University of California, Berkeley, USA (31.05.–03.06.2016)
ICII-2016, Marburg: "Interaction and correlation effects at ultimately thin interfaces: atomically thin quasi-2D crystals"

Dr. Stefan Mathias, Georg-August-Universität Göttingen (31.05.–03.06.2016)
ICII-2016, Marburg: "Spin filtering at a Bi superstructure on Au(111) interface"

Prof. Dr. Henning Riechert, Paul-Drude-Institut für Festkörperelektronik, Berlin (31.05.–03.06.2016)
ICII-2016, Marburg: "Growth of two-dimensionally bonded materials – fiction, facts and surprises"

Prof. Dr. Michael Rohlfing, Westfälische Wilhelms-Universität Münster (31.05.–03.06.2016)
ICII-2016, Marburg: "Electronic spectra of layered materials and monolayer adsorbates"

Dr. Julia Stähler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (31.05.–03.06.2016)
ICII-2016, Marburg: "Charge carrier and exciton dynamics at hybrid inorganic/organic interfaces"

Prof. Dr. F. Stefan Tautz, Peter Grünberg Institut, FZ Jülich (31.05.–03.06.2016)
ICII-2016, Marburg: "The backside of graphene"

Dr. Ursula Wurstbauer, TU München (31.05.–03.06.2016)
ICII-2016, Marburg: "Light matter interaction, exciton-phonon coupling and optoelectronic properties in TMDCs"

Prof. Dr. Yoshiyasu Matsumoto, Kyoto University, Japan (31.05.2016)
ICII-2016, Marburg: "Structures of water at interfaces of ice crystal films grown on metals"

Prof. Dr. Hrvoje Petek, University of Pittsburgh, USA (01.06.2016)
ICII-2016, Marburg: "Plasmonically enhanced multiphoton photoemission at metal nanoparticle decorated surfaces"

Prof. Dr. Toshiaki Munakata, Osaka University, Japan (02.06.2016)
ICII-2016, Marburg: "Unoccupied electronic structures of rubrene: from evaporated films to single crystals"

Dr. Kunie Ishioka, National Institute for Materials Science, Tsukuba, Japan (03.06 2016)
ICII-2016, Marburg: "Ultrashort acoustic pulses generated at buried GaP/Si interfaces"

Prof. Dr. Christopher J. Stanton, University of Florida, Gainesville, USA (03.06.2016)
ICII-2016, Marburg: "Ultrafast coherent optical phonon probing of electronic properties of surfaces and interfaces"

Prof. Dr. Thomas H. Seligman, Universidad Nacional Autónoma de México (09.06.2016)
"Halls theory of degeneracy in the Hückel model, group-theoretical considerations and model experiments"

Dr. Taka Ueba, Institute of Molecular Science, Okazaki, Japan (08.06.2016)
"Absorption configuration and molecular orbital energy rearrangement by organic–metal interaction"

Dr. Frederik M. Schiller, Centro de Física de Materiales, San Sebastián, Spain (08.07.2016)
"Electronic structure of the TiOPc-PTCDA interface"

Dr. François C. Bocquet, Peter Grünberg Institut, FZ Jülich (15.09.2016)
"Two approaches to probe internal interfaces: phonon dispersion and chemically resolved atomic structure measurements"

Dr. François Rochet, LCPMR, Université Pierre et Marie Curie, Paris, France (07.10.2016)
"Chemical reactions at silicon surfaces using STM and (time-resolved) XPS in combination"

Prof. Dr. David C. Johnson, University of Oregon, Eugene, USA (24.10.2016)
"Heterostructures with designed nano-architecture: synthesis via kinetic control and systematic trends in physical properties"

Prof. Dr. Martin Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (03.11.2016)
"Ultrafast excited state dynamics and nonlinear optical spectroscopy at interfaces"

Prof. Dr. Alfred Meixner, Eberhard Karls Universität Tübingen (17.11.2016)
"Tip enhanced near-field optical spectroscopy: from fundamentals to applications"

Prof. Dr. Francisco Guinea, Madrid Institute for Advances Studies, Spain and University of Manchester, UK (08.12.2016)
"Strains and electrons in two-dimensional materials"

Dr. Ruslan Temirov, Peter Grünberg Institut, FZ Jülich (09.12.2016)
"Charging of a single-molecule quantum dot fixed to the tip of a scanning probe microscope: Insights from the force measurements"

Dr. Klaus Stallberg, TU Clausthal (09.12.2016)
"Spectromicroscopy of thin porphyrin films and their interaction with plasmonic silver structures"

Prof. Dr. Eike Schwier, Hiroshima University, Hiroshima Synchrotron Radiation Center, Japan (19.12.2016)
"Insights into the geometric and electronic surface structure of the topological insulator $TlBiSe_2$"

2017

Prof. Dr. Eleonora Backus, Max-Planck-Institut für Polymerforschung, Mainz (16.01.–18.01.2017)
Winter School, Rauischholzhausen: "Towards understanding the mechanism of water splitting on TiO_2"

Prof. Dr. Alexey Chernikov, Universität Regensburg (16.01.–18.01.2017)
Winter School, Rauischholzhausen: "Exciton physics of semiconducting 2D materials"

Dr. Matteo Gatti, École Polytechnique, Paris, France (16.01.–18.01.2017)
Winter School, Rauischholzhausen: "Exciton band structure in two-dimensional materials"

Dr. Christian Papp, Friedrich-Alexander Universität Erlangen-Nürnberg (16.01.–18.01.2017)
Winter School, Rauischholzhausen: "In-situ Studies of the Reactivity of Model Catalysts: Surface Chemistry from flat surfaces to nanoparticles"

Dr. Katrin Siefermann, Leibniz Institut für Oberflächenmodifizierung, Leipzig (16.01.–18.01.2017)
Winter School, Rauischholzhausen: "Exciton physics of semiconducting 2D materials"

Prof. Dr. Andreas Görling, Friedrich-Alexander Universität Erlangen-Nürnberg (26.01.2017)
"Carbon-rich two-dimensional materials and their interaction with surfaces: insight from theory"

Prof. Dr. Meike Stöhr, University of Groningen, Netherlands (09.02.2017)
"Structural and electronic properties of (supra)molecular assemblies on surfaces"

Prof. Dr. John F. Corrigan, Western University, London, Canada (08.03.2017)
"Assembly of Metal-Chalcogenide Clusters using NHC Ligands"

Prof. Dr. Charles Campbell, University of Washington, USA (30.03.2017)
"Thermodynamics and kinetics of elementary reaction steps on late transition metal surfaces"

Prof. Dr. Maki Kawai, University of Tokyo, Japan (02.05.2017)
"Chemical reactions at surfaces: single molecular view"

Prof. Dr. Sabine Maier, Friedrich-Alexander Universität Erlangen-Nürnberg (02.05.2017)
"On-surface synthesis and electronic properties of molecular networks"

Prof. Dr. Jin Zhao, University of Science and Technology, Hefei, China (08.06.2017)
"Nonadiabatic molecular dynamics investigation on the ultrafast carrier dynamics at interfaces"

Prof. Dr. Rupert Huber, Universität Regensburg (11.06-16.06.2017)
USD-10, Inzell: "Lightwave Electronics in Layered Semiconductors and single Molecules"

Dr. Kenta Kuroda, University of Tokyo, Japan (11.06-16.06.2017)
USD-10, Inzell: "Optical Control over Spin-Polarized Surface States in Topological Insulators"

Prof. Dr. Toshiaki Munakata, Osaka University, Japan (11.06-16.06.2017)
USD-10, Inzell: Session Chair

Prof. Dr. Hrvoje Petek, University of Pittsburgh, USA (11.06-16.06.2017)
USD-10, Inzell: "Ultrafast Coherent Multidimensional Multiphoton Photoemission Spectroscopy"

Prof. Dr. Jin Zhao, University of Science and Technology, Hefei, China (11.06-16.06.2017)
USD-10, Inzell: "Phonon Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface"

Prof. Dr. Pedro M. Echenique, Donostia International Physics Center, San Sebastián, Spain (06.07.2017)
Kick-Off Meeting: "The Sublime Utility of Useless Science"

Prof. Dr. Rolf Haug, Leibniz Universität Hannover (13.07.2017)
"Twisted bilayers of folded graphene"

Prof. Dr. Susan E. Babcock, University Wisconsin-Madison, USA (23.07-26.07.2017)
"Growth and Stability of $GaAs_{1-x}Bi_x$ and Related Metastable Materials: Insights Gained from the Microstructure and More"

Prof. Dr. Zoe L. Bushell, University of Surrey, UK (23.07-26.07.2017)
"Bismide alloys for device applications"

Prof. Dr. Joanna Millunchick, University of Michigan, USA (23.07-26.07.2017)
"Surface-Mediated Compositional Inhomogeneities in GaAsBi Alloys"

Prof. Dr. Eoin O'Reilly, University College Cork, Ireland (23.07-26.07.2017)
"Band mixing and localisation effects in semiconductor alloys"

Dr. Ryuchi Arafune, National Institute for Materials Science, Tsukuba, Japan (05.09.2017)
"Spintexture in image potential states and its application to opto-spintronics"

Dr. Shunsuke Tanaka, Kyoto University, Japan (20.10.2017)
"Optical response of π conjugated materials"

Dr. Kento Uchida, Kyoto University, Japan (06.11.2017)
"Time- and space-resolved THZ-induced luminescence in GaAs"

Dr. Frank Ortmann, TU Dresden (08.11.2017)
"Organic Semiconductors and Interfaces: Fundamentals for Applications"

Dr. Claudia Rödl, Friedrich-Schiller-Universität Jena (08.11.2017)
"Electronic Excitations in Matter from First Principles: From 3D towards 2D Systems"

Dr. Stefan Schulz, Tyndall National Institute, Cork, Ireland (08.11.2017)
"Carrier localization effects in III-N alloys and heterostructures: Impact of random alloy fluctuations and interface roughness"

Dr. Stefan Wippermann, Max-Planck-Institut für Eisenforschung, Düsseldorf (08.11.2017)
"Light-Matter Interactions at Interfaces: From Analysis Techniques to Applications in Solar Energy Conversion"

Prof. Dr. Christoph Tegenkamp, TU Chemnitz (16.11.2017)
"Epitaxial graphene nanostructures for future carbon based electronics"

Prof. Dr. Armin Gölzhäuser, Universität Bielefeld (14.12.2017)
"Fabrication and Application of 2D Carbon Materials"

2018

Dr. Oliver MacLean, University of Toronto, Canada (22.01.2018)
"Reaction Dynamics of Hot Molecules at Surfaces"

Prof. Dr. Ulrich Heinzmann, Universität Bielefeld (01.02.2018)
"Attosecond delays in photoemission and their relation to phase resolved photoelectron spectroscopy"

Dr. Suguru Ito, University of Tokyo, Japan (07.02.2018)
"Revealing electronic properties of semimetal bismuth via the systematic modulation on the nanoscale"

Prof. Dr. Ermin Malic, Chalmers University of Technology, Gothenborg, Sweden (06.03.–09.03.2018)
WUPCOM'18, Winklmoosalm: "Dark exciton dynamics in atomically thin 2D nanomaterials"

Dr. Marcel Reutzel, University of Pittsburgh, USA (20.04.2018)
"High-Order multiphoton photoemission from noble metal surfaces"

Prof. Dr. Alfred Leitenstorfer, Universität Konstanz (26.04.2018)
"Subcycle Quantum Physics of Electrons and Photons"

Prof. Dr. Alexander Tkatchenko, Université du Luxembourg (03.05.2018)
"First-Principles Modeling of Molecular Polymorphism in Crystals and on Surfaces"

Prof. Dr. Joachim Wagner, Fraunhofer Institut für Angewandte Festkörperphysik, Freiburg (17.05.2018)
"Quantum Cascade Lasers for Spectroscopy – Concepts and Use Cases"

Prof. Dr. Peter Zeppenfeld, Johannes Kepler Universität Linz, Austria (24.05.2018)
"Optical spectroscopy of surfaces, thin films and nano-structures"

Prof. Dr. Ralph Claessen, Justus-Maximilians-Universität Würzburg (07.06.2018)
"Topological insulators go elemental"

Prof. Dr. Ewan M. Wright, University of Arizona, Tucson, USA (21.06.2018)
"A brief history of optical filamentation in strong field light propagation: from recurrent collapse to megafilaments"

Prof. Dr. Akio Kimura, Hiroshima University, Japan (20.07.2018)
"Magnetically doped topological insulators"

Prof. Dr. Mats Fahlman, Linköping University, Sweden (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Ternary organic bulk heterojunction solar cells"

Prof. Dr. Satoshi Kera, Chiba University, Japan (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Evolution of electron localization upon assembling the molecules on the surface"

Prof. Dr. Jiong Lu, National University of Singapore (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Recent STM studies of single molecule and defect in gated 2D material devices"

Prof. Dr. Masahiro Shibuta, Keio University, Yokohama, Japan (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Spectroscopy and imaging of photocarriers in organic functional films probed by two-photon photoemission"

Prof. Dr. Petra Tegeder, Universität Heidelberg (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Formation of occupied and unoccupied hybrid bands at interfaces between metals and organic molecules"

Prof. Dr. Yoishi Yamada, University of Tsukuba, Japan (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Exploring the structure-property relationships of the well-ordered organic films"

Prof. Dr. Jun Yoshinobu, University of Tokyo, Japan (23.10.–26.10.2018)
ASOMEA-IX, Schluchsee: "Gas exposure effects on monolayer pentacene FET studied by using non-invasive GaIn probes"

Prof. Dr. Masahiro Shibuta, Keio University, Yokohama, Japan (29.10.2018)
"Photocarrier dynamics in organic functional films studied by two-photon photoemission spectroscopy and microscopy"

Prof. Dr. Takashi Yamada, Osaka University, Japan (29.10.2018)
"Spectroscopic and microscopic investigations of unoccupied states at the organic/substrate interface"

Prof. Dr. Michael Horn-von Hoegen, Universität Duisburg-Essen (08.11.2018)
"Watch the atoms moving: Femtosecond ultrafast electron diffraction at surfaces"

Prof. Dr. Gerd Schönhense, Johannes-Gutenberg-Universität Mainz (29.11.2018)
"Multidimensional photoemission data recording"

Prof. Dr. Kai Roßnagel, Christian-Albrechts-Universität zu Kiel (13.12.2018)
"Femto-stroboscopic photoemission of quantum materials: From the extreme ultraviolet to hard X-rays"

2019

Dr. Kunie Ishioka, National Institute for Materials Science, Tsukuba, Japan (04.02.2019)
"Coherent oscillations at GaP/Si(001) Interfaces under below-bandgap photoexcitation"

Prof. Dr. David C. Johnson, University of Oregon, Eugene, USA (12.02.2019)
"Controlling Solid State Reaction Pathways to Synthesize Targeted Metastable Compounds"

Prof. Dr. Masahiro Shibuta, Keio University, Yokohama, Japan (10.05.2019)
"Photoexcited state dynamics at functional thin films fabricated with organic molecules and nanoclusters"

Prof. Dr. Katsumi Tanimura, Osaka University, Japan (13.05.2019)
"Excitonic signatures in time- and angle-resolved photoemission from semiconductors"

Prof. Dr. Yoshihiro Miyauchi, National Defense Academy, Kanagawa, Japan (15.05.2019)
"Optical second harmonic generation microscopy and spectroscopy of mono- and few-layer dichalcogenides TX_2 (T=Mo, W, X=S, Se)"

Dr. Suguru Ito, University of Tokyo, Japan (17.05.2019)
"Electronic properties of bismuth studied by systematic film control at the nanoscale"

Prof. Dr. Markus Mauerer, Hochschule für Angewandte Wissenschaften, München (20.05.2019)
"From Laser Spectroscopy of Surfaces to Teaching Engineering and Management Students – Career, Tasks and Options of a Professor at an University of Applied Sciences"

Prof. Dr. Moritz Sokolowski, Rheinische Friedrich-Wilhelms-Universität, Bonn (23.05.2019)
"The hexagonal boron nitride layer on Cu(111) as an ultrathin spacer layer for functional molecules"

Prof. Dr. Willi Auwärter, TU München (06.06.2019)
"Functional molecules and 2D materials: interface characterization, intercalation, and on-surface reactions"

Prof. Dr. Jerry V. Moloney, University of Arizona, Tucson, USA (17.06.2019)
"Ultrafast Carrier Scattering Effects in CW and Pulsed VECSELs: From W-Lasers to Offset-Free Mid-IR Frequency Combs"

Dr. Kenta Kuroda, University of Tokyo, Japan (17.07.2019)
"Observation of a week topological insulator state by nano-ARPES"

Dr. Zhonghui Nie, Nanjing University, China (19.08.2019)
"Photocarrier dynamics of 2D TMDs and their heterostructures"

Dr. Kevin Dorney, University of Colorado Boulder, USA (16.09.2019)
"A twist in strong-field physics: structured EUV beams and attosecond pulses for nanoscale spectroscopy and imaging"

Dr. Christoph Kastl, TU München (15.10.2019)
"Ultrafast optoelectronics in materials with topological order"

Dr. Gustav Bihlmayer, Peter Grünberg Institut, FZ Jülich (16.10.2019)
"Two-dimensional magnetic topological materials: insights from DFT"

Prof. Dr. Michael Heuken, RWTH Aachen (16.10.2019)
"Application, growth and characterization of 2D nanomaterials"

Dr. Marcel Reutzel, Georg-August-Universität Göttingen (18.10.2019)
"Dressing metallic surface bands with ultrafast optical fields"

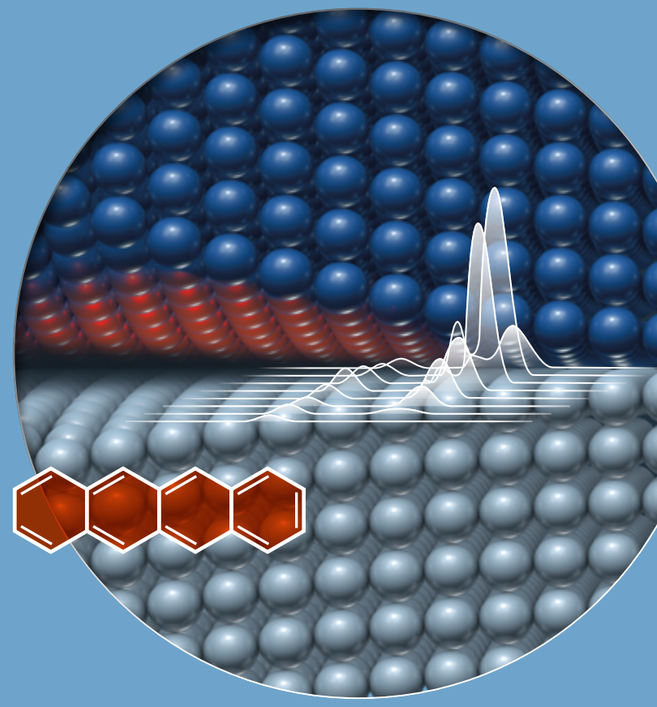
Prof. Dr. Jerome Cornil, Université de Mons, Belgium (05.12.2019)
"Theoretical insight into electronic processes at hybrid interfaces in opto-electronic devices"

Dr. Reinhard Maurer, University of Warwick, UK (10.12.2019)
"Computational insights into light- and electron-driven chemistry at surfaces"

Prof. Dr. Kyoko Ishizaka, University of Tokyo, Japan (17.12.2019)
"Ultrafast nematic excitation in FeSe superconductor"

Dr. Jenny Clark, University of Sheffield, UK (19.12.2019)
"Singlet fission in organic semiconductors"

FACTS AND NUMBERS



SFB 1083 in Numbers

Funding DFG	1st Funding Period	2nd Funding Period
Salaries		
Postdocs	1.164.500	1.231.200
Doctoral Candidates	3.224.000	4.557.600
Non-research staff	120.000	141.600
Student Assistants	146.300	184.800
	4.654.800	6.115.200
Direct costs		
Consumables and instrumentation	1.585.900	1.169.000
Core Support	1.027.000	1.435.500
	2.612.900	2.604.500
Overheads	1.453.400	1.918.800
Overall Funding DFG	8.721.100	10.638.500

Staff positions funded by DFG	1st Funding Period	2nd Funding Period
Postdocs	5	4
Doctoral Candidates	20	24
Non-research staff	1	2
Student Assistants	7	7
	33	37

Standard research equipment	1st Funding Period	2nd Funding Period
Federal and state large infrastructure programme	3.286.000	1.800.000
Direct costs Philipps-Universität Marburg	489.400	574.400
Direct costs other institutions	24.000	96.000

Staff funded by university & DFG	1st Funding Period	2nd Funding Period
Principal Investigators	19	24
hereof Junior Research Group Leaders	2	6
Associated Members	7	8
Postdocs	12	10
Doctoral Candidates	40	46
Research Staff	2	5
Non-research staff	31	36
MSc-Students	19	26
Student Assistants	9	14

Publications	2013–2019
Total	255
Contributions by 2 subprojects	77
Contributions by 3 subprojects	26
Doctoral Dissertations	52

Scientific exchange	2013–2019
International conferences and symposia organized	10
Internal workshops	29
Colloquia and seminars organized	102
SFB-invited speakers	225
Guest Scientists	76
International conferences attended	191
Invited talks presented by SFB-staff	105

Also	2013–2019
Research prizes and honors	31
Appointments of SFB-staff as professors	8

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Structure and Dynamics
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