TECHNISCHE UNIVERSITÄT
CHEMNITZ

Faculty of Natural Science

ICSFS 18

International Conference on Solid Films and Surfaces

August 28 - September 02, 2016
in Chemnitz, Germany

Abstract - Book

(with space for your notes)

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Impressum

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Technology at TU Chemnitz

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Welcome Address

Dear Colleagues,

welcome to Chemnitz! The city, more than 800 years old, is situated in the heart of Saxony and is the third-largest in the new Federal States; about 245,000 people live here. Fascinating architecture reflects the changing times and spirit of those things which have shaped the city: industrial monuments, redeveloped Gründerzeit residential quarters such as the Kassberg, Villa Esche or the city centre, which has been completely modified since Re-unification, bridge the gap from yesterday to today and tomorrow. Just as famous is the 7.10-metres-high Karl-Marx bust made of bronze by Lew Kerbel in 1971, locally known as "Nischel" (head).

Probably no other city in Germany fits the description "City of Modernity" quite so well as Chemnitz does. Developed at the time of Classical Modernism, which still gives impetus to the development of business and science, the influences of the cultural and architectural Modernism are visible and perceptible. In 2006, the new centre was awarded the DIFA award for inner-city quarters for its successful mixture of retail, offices, catering trades, residential areas, leisure activities, and culture.

Chemnitz is a capital of culture. The city theatre is nationally and internationally prized along with the Opera House and the Playhouse with exceptional productions as well as the Robert-Schumann Philharmonic Orchestra. The City Art Collections on Theaterplatz are regularly included in the Federal German feature pages with their exhibitions. Moreover, one of the largest private German art collections found its place in Chemnitz in 2007: In the Gunzenhauser Museum almost 2,500 eminent works await the visitors in a former Sparkasse building. The works are of the Classic Modernism period, the art between the World Wars and the second half of the 20th century, among which is one of the largest Otto-Dix collections worldwide.

Chemnitz was, and still is, a city with a flourishing economy and inventive talent. And Chemnitz today is once again a competitive centre for technological innovation, for which it owes its numerous entrepreneurs and their proximity to the research centres. Since 2004, Chemnitz has been counted among the ten strongest growing cities of Germany every year.

Situated in the center of the Chemnitz “Wissenschaftsregion” (“science region”), the Technische Universität (TU) Chemnitz is home to more than 11,000 students from 90 countries. With approximately 2,300 employees in science, engineering, and management, the TU Chemnitz is among the most important employers in the region. Today, TU Chemnitz stands for outstanding research. Within the core competencies “Materials and Smart Systems”, “Resource-efficient Production and Lightweight Structures” and “Humans and Technology”, solutions for the challenges of tomorrow are developed. The profile of TU Chemnitz is characterized by a unique constellation of competencies across eight faculties. Thanks to this constellation, Chemnitz is emerging as an internationally visible research hub for future value creation processes and sustainable growth for the future.

Within the core competency “Materials and Smart Systems”, scientists at the TU Chemnitz are, for instance, involved in the Federal Cluster of Excellence “Center for Advancing Electronics Dresden” (cfAED). Several DFG Research Groups (Towards Molecular Spintronics, Sensorical Micro- and Nanosystems, and Twin Poymerisation) composed of physicists, chemists, and engineers work in the field nanotechnology. In addition, TU Chemnitz will be the home of the “Center for Materials, Architectures and Integration of Nanomembranes” (MAIN), which is unique in Europe.

The Faculty of Natural Science as a faculty with strong connections between the Institute of Chemistry and the Physics Institute on the basis of experimental and theoretical methods is devoted both to fundamental research as well as applied science. The faculty concentrates on the following four research topics: Complex Materials, Molecular Systems, Scientific Modelling and Simulation, and Sensors and Cognition. Traditionally, research in the Institute of Physics was and still is focused on condensed matter systems and, in particular thin films and surfaces. Even well before reunification Physics in Chemnitz was well-recognised for the work on e.g. hard coatings. Later this work was continued and strongly extended in large-scale projects like “Thin Films and Non-Crystalline Materials”, “Methods and Materials for the Nanometer Scale”, “Micromechanical Sensor and Actor Arrays”, or the “Nano System Integration Network of Excellence”. Today two-dimensional materials like graphene and transition metal dichalcogenides and low-dimensional materials such as carbon nanotubes and semiconductor quantum dots belong to the research interests in the Institute of Physics. We are proud of an excellent infrastructure and you are all welcome to visit our facilities in the Physics building which was opened in 2008.

The International Conference on Solid Films and Surfaces (ICSFS) has taken place since 1978, gathering an increasing number of scientists from all over the world. The 18th edition, which will take place in Chemnitz (Germany) from August 28th to September 2th 2016, follows the previous meetings held in Tokyo (1978), Washington (1981), Sydney (1984), Hamamatsu (1987), Providence (1989), Paris (1992), Hsinchu (1994), Osaka (1996), Copenhagen (1998), Princeton (2000), Marseille (2002), Hamamatsu (2004), Bariloche (2006), Dublin (2008), Beijng (2010), Genoa (2012), and Rio (2014).

ICSFS 18 in Chemnitz focuses on recent advances in controlling and characterizing the physical and chemical properties of films and surfaces, with a particular emphasis on materials for electronic, photonic and spintronic applications, in addition to bio-functionalized structures and devices ICSFS is strongly interdisciplinary, covering also nano and nano-bio science and technology and metrology, wherever surfaces are involved in the future devices. There are 5 plenary talks, 43 invited talks as well as 50 oral and 60 poster contributions. Enjoy the scientific and the social program with the excursion to Augustusburg!

Chemnitz, August 2016

Thomas Seyller and Dietrich RT Zahn

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- **for Talks:**

The venue of the ICSFS 18 conference is the Central Lecture Hall Building on the campus.
Address: Reichenhainer Str. 90, 09126 Chemnitz, near bus stop line 51.

We provide a notebook with Win10, MS Office 2013, and Adobe Acrobat 11. If you will use your own computer please connect your computer prior to the session and check whether your presentation works properly. As video connection is available VGA and a HDMI connection.
In case of questions please contact our technical team or
call ☎ **+49 371 531-29884** or ☎ **+49 151 11 64 28 90**.

- **for Posters:**

The poster boards have the size DIN A0 (vertical: 841 mm x 1189 mm). The poster session will take place in the 1st floor in the Central Lecture Hall Building. Please leave your poster at the registration desk until the lunch break on Monday. We will fix all posters on the boards. On Friday morning the posters will be removed.

- **Excursion and Conference Dinner:**

We will go by bus to Augustusburg Castle and visit a falconer's show. Afterwards there is the possibility to visit one of the museums in the castle.
(↗ http://www.die-sehenswerten-drei.de/de/Augustusburg/Schloss-Augustusburg_1229.html)

Before the conference dinner in the castle restaurant you are invited to an organ concert in the castle chapel.

After the conference dinner we will all return by bus to Chemnitz.

- **for WLAN:**

Access to WLAN is available in the entire Central Lecture Hall Building. Two nets are available: >eduroam< (login with the access data of her institute) and >special-hsg< (conference WLAN, PSK: icsfs18chemnitz).

- **Contacts:**

If you have any problems or trouble please contact our support team at the registration desk or call one of the following numbers:

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Program Overview

28th August - Sunday		
16:00 - 19:00	Registration	Organization Office N106
18:00 - 22:00	Get Together	Lecture Hall Building

29th August - Monday				
07:30 - 08:45	Registration			Organization Office N106
08:45 - 09:15	Opening session			N112
09:15 - 10:00	C. Wöll			
10:00 - 10:30	Coffee break			
10:30 - 11:00	P. Jelinek			
11:00 - 11:30	A. Cricenti			
11:30 - 12:00	J. Jobst			
12:00 - 13:30	Break for lunch			
13:30 - 14:00	M. Thelakkat	N112	R. Berndt	N113
14:00 - 14:15	E. Zenkevich		V. M. Silkin	
14:15 - 14:30	O. Stroyuk		E. V. Chulkov	
14:30 - 14:45	A. G. Milekhin			
14:45 - 15:15	Coffee break		Coffee break	
15:15 - 15:30	O. Hellwig		R. D. Rodriguez	
15:30 - 15:45			A. Pucci	
15:45 - 16:00	H. Ibach		K. Pedersen	
16:00 - 16:15	B. Buechner		B. S. Mendoza	
16:15 - 16:30			E. Bortchagovsky	
16:30 - 16:45			P. H. Thiesen	
16:45 - 17:00	IOP Publishing			

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09:45- 10:15	S. Kera	N112	J. S. Speck	N113
10:15 - 10:45	Coffee break		Coffee break	
10:45 - 11:00	N. Esser		J. F. Woitok	
11:00 - 11:15	R. Schlesinger		B. Borkenhagen	
11:15 - 11:30	T. Sakurai		U. Rossow	
11:30 - 11:45	P. Amsalem		E. Pincik	
11:45 - 12:00	D. A. Evans		N. Tolk	
12:00 - 13:30	Break for lunch			
13:30 - 14:00	S. Kowarik	N112	M. Wuttig	N113
14:00 - 14:15	B. Höffling		Yu. M. Azhniuk	
14:15 - 14:30	M. Reutzel		P. H. Thiesen	
14:30 - 14:45	T. L. Einstein		R. Calarco	
14:45 - 15:00	K. Bobrov			
15:00 - 15:30	Coffee break		Coffee break	
15:30 - 15:45	M. Scheele		S. Murakami	
15:45 - 16:00	M. Grundmann			
16:00 - 16:15			C. M. Acosta	
16:15 - 16:30	I. Arnay		K. Schouteden	
16:30 - 16:45	P. S. N. Barimar		A. Kimura	
16:45 - 17:00	C. Schmidt			
17:00 - 18:30	Poster session			Foyer Lecture Hall Building

31st August - Wednesday	N112	N113
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09:45 - 10:15	S. Facsko	P. Hofmann
10:15 - 10:45	Coffee break	Coffee break
10:45 - 11:00	U. Kreibig	J.-M. Layet
11:00 - 11:15	D. Erb	P. H. Thiesen
11:15 - 11:30	R. Zdyb	Z. Khan
11:30 - 11:45	I. Miccoli	C. Papp
11:45 - 12:00	H. Holtgrewe	
12:00 - 12:15	Z. Li	K. L. Syres
12:15 - 14:00	Break for lunch	
14:00 - 18:00	Excursion - Augustusburg	
18:00 - 22:00	Social dinner	

1st September - Thursday	N112	N113	
09:00 - 09:45	E. Malic		09:00 - 09:45
09:45 - 10:15	M. Smerieri	Opening - D. R. T. Zahn S. Kiyatskaya	09:45 - 09:55 09:55 - 10:20
10:15 - 10:45	Coffee break	Coffee break	10:20 - 10:45
10:45 - 11:00	A. Matkovic	T. Rüffer	10:45 - 11:10
11:00 - 11:15	C. Tegenkamp		
11:15 - 11:45	W. Auwärter	T. Hahn	11:10 - 11:35
11:45 - 12:00		V. Kataev	11:35 - 12:00
12:00 - 13:30	Break for lunch		12:00 - 13:30
13:30 - 14:00	L. Kühl Teles	C. Hess	13:30 - 13:55
14:00 - 14:15	D. A. Evans	M. Hietschold	13:55 - 14:20
14:15 - 14:30	T. Seyller		
14:30 - 14:45	S. Shah	S. Tatay	14:20 - 14:45
14:45 - 15:00	C. Noguez	P. F. Siles	14:45 - 15:10
15:00 - 15:30	Coffee break	Coffee break	15:10 - 15:30
15:30 - 15:45	C. Wagner	M. Knupfer	15:30 - 15:55
15:45 - 16:15	A. V. Krasheninnikov	G. Salvan	15:55 - 16:20
16:15 - 16:45	A. C. Ferrari	H. Prima-Garcia	16:20 - 16:45
16:45 - 17:00		F. Zhu	16:45 - 17:10
17:00 - 18:30	Poster session	Foyer Lecture Hall Building	17:10 - 18:30

2nd September - Friday	N112
09:00 - 09:30	H.-P. Steinrück
09:30 - 10:00	B. Kersting
10:00 - 10:30	Coffee break
10:30 - 11:00	C. Kumpf
11:00 - 11:45	R. Wiesendanger
11:45 - 12:15	Closing session

List of Oral Sessions & Abstracts

Sunday:

16:00 – 19:00	Registration
18.00 – 22:00	Get Together

Monday:

07:30	Registration
	N112
08:45	Opening session
09:15	*Plenary Talk*: C. Wöll
10:30	*Invited Talk*: P. Jelínek
11:00	*Invited Talk*: A. Cricenti
11:30	*Invited Talk*: J. Jobst

	N112		N113
13:30	*Invited Talk*: M. Thelakkat	13:30	*Invited Talk*: R. Berndt
14:00	E. Zenkevich	14:00	V. M. Silkin
14:15	O. Stroyuk	14:15	*Invited Talk*: E. V. Chulkov
14:30	A. G. Milekhin		
15:15	*Invited Talk*: O. Hellwig	15:15	R. D. Rodriguez
		15:30	A. Pucci
15:45	H. Ibach	15:45	K. Pedersen
16:00	*Invited Talk*: B. Buechner	16:00	B. S. Mendoza
		16:15	E. Bortchagovsky
		16:30	P. H. Thiesen

16:45 IOP Publishing (N113)

PROGRAMMED ASSEMBLY OF MOLECULAR FRAMEWORKS: A NEW CLASS OF DESIGNER SOLIDS?

Christof Wöll

Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), FRG

The demand for advanced materials with novel combinations of different functionalities requires the development of new types of solids. Self-assembly of one or different types of functional molecular units can be employed to fabricate crystalline arrangements, yielding complex but at the same time structurally well defined, highly ordered “Designer Solids”, which exhibit functionalities going well beyond that provided by the individual building blocks.

In this presentation, it will become evident that a recently introduced class of supramolecular materials, metal-organic frameworks, or MOFs, carry an enormous potential with regard to the fabrication of solids with unusual physical properties [1]. MOFs are stable materials, with decomposition temperatures well above 200°C (in some cases > 500°C). With selected examples, we will demonstrate the interesting, and often surprising (e.g. negative thermal expansion coefficient), mechanical, electronic, magnetic and optical properties of these molecular, crystalline materials.

We have developed a liquid phase epitaxy (LPE) process, which allows growing MOFs on modified substrates using a layer-by-layer procedure [1]. For the cm-sized, highly oriented MOF thin films with thickness in the micrometer-regime basic physical properties (mechanical [2,7], optical [3], electronic [4], magnetic [5]) of these porous, molecular solids can be determined using standard methods.

The porous nature of these crystalline solids opens up the prospect of adding additional functionality by placing molecules [8] or nanoobjects inside the voids within the MOFs, e.g. metal clusters or dye molecules [9].

Keywords: Designer Solids, Metal-Organic Frameworks, Organic Thin Films

References

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HIGH-RESOLUTION AFM/STM IMAGES: BEYOND IMAGING

P. Jelínek[a]

[a] Institute of Physics of CAS, Cukrovarnicka 10, Prague, Czech Republic

High-resolution AFM/STM images of molecules acquired functionalized tips [1,2] created a lot of excitement among researchers from many fields including material science, physics and chemistry. So far, the method has been mostly used to visualize chemical structures of molecules on surfaces, but quantitative information is mostly missing. Further proliferation of the technique depends critically on our ability to extract novel information or characterize/identify complex molecular structures.

In this talk, we will address both questions. First we will discuss a novel technique that maps out the electrostatic potential over a single molecule with unprecedented resolution [3]. The technique exploits the fact that image distortions typically observed in high-resolution atomic force microscopy images are for a significant part due to the electrostatic force acting between the tip and the charge distributed in the molecule of interest [4]. In addition, we report sub molecular resolution of water clusters achieved with AFM, which indicates that the H-bonded water systems remain intact during the high-resolution AFM imaging. What more, the AFM images provide information about chiral character of the electrostatic field of the water clusters.

In the second part, we will exploit the high-resolution images to identify the individual chemical products of on-surface reaction. What more, we will demonstrate chirality transfer from a homochiral helical precursor to enantiofacially adsorbed prochiral products through a cascade of stereoconservative on-surface reactions (see Fig.). We believe that the possibility to form globally enantiopure assemblies of prochiral molecules through on-surface synthesis opens a new way of expressing 2D chirality in so far unexplored types of organic-inorganic chiral surfaces.

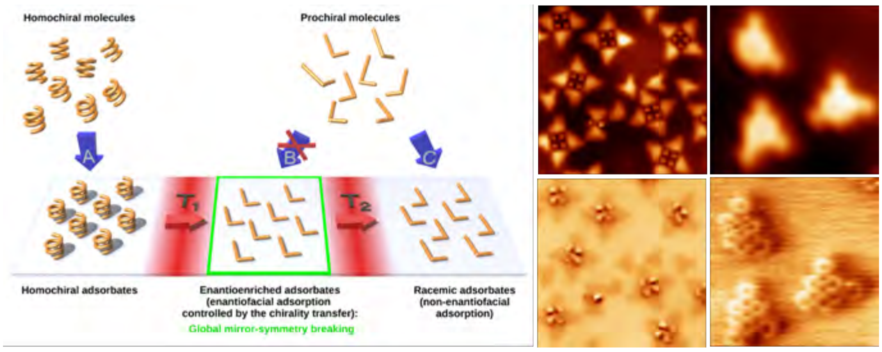

Fig. Right: The proposed concept of global mirror-symmetry breaking in the system of prochiral molecules on an achiral substrate through controlled on-surface chemistry reaction. Left: High-resolution AFM/STM images of different products of the chemical reaction.

Keywords: AFM; STM; Chirality; water; electrostatic field; DFT; sub molecular resolution

References

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[2] L. Gross et al, Science 325 (2009) 1110.
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SNOM SPECTROSCOPY FOR TISSUE IMAGING AND CANCER DIAGNOSTICS

A. Cricenti[a]* , M. Luce[a], M. Ortenzi[a], M.R.F. Siggel-King[b], T. Craig[b], J. Ingham[b], D. Martin[b], P. Weightman[b]

[a]Istituto di Struttura della Materia (ISM-CNR), 00133 Rome, Italy
[b]Department of Physics, University of Liverpool, Liverpool L69 7ZE, United Kingdom

We present a fully implemented Infrared (IR) Scanning Near-field Optical Microscopy (SNOM) in spectroscopic mode for tissue imaging and early cancer diagnostics. The SNOM has been coupled with an infrared light source, based on Free Electron Laser at the ALICE facility in Daresbury [1]. The potential of IR spectroscopy to characterise cancerous tissues has long been recognised and studies of various cancers by many groups have established that regions of malignant tissue can be easily identified on the basis of its IR spectrum. The oesophageal adenocarcinoma, the cancer with the fastest rise in incidence in the Western world, requires an instrument providing specific chemical images at sub-cellular level of oesophagus tissue.

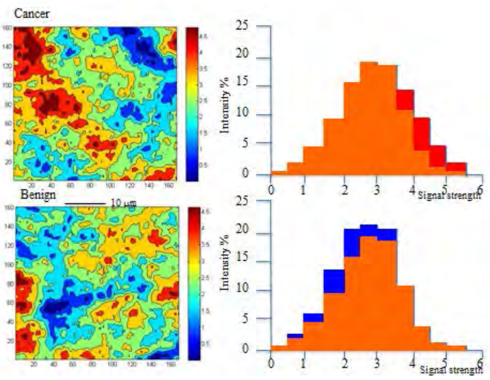

Fig. 1. IR-SNOM image maps .

Preliminary results of IR-SNOM on oesophageal adenocarcinoma have shown that the system can operate at nanometer resolution and has been able to distinguish between healthy and malignant tissues [2]. The optical fibre has been driven in particular areas of the oesophageal tissue and topographical and optical images have been collected simultaneously at different wavelengths. In particular, SNOM images were collected at wavelengths of 7.0 μm (no strong biomarker), 7.3 μm (protein/glycoprotein), and 8.05 μm (DNA). Figure 1 shows 40 μm x 40 μm optical SNOM images for two samples, labelled Cancer and Benign: the colour maps show the location of intense DNA (red), intense protein/glycoprotein (blue) and of strong overlap of DNA and protein/glycoprotein (orange). As clearly visible, Cancer sample shows a large spread of intense signal from DNA whereas Benign sample shows a lower overall density of DNA, which is more dispersed and exhibits more localised centres. This approach demonstrates the potential of the IR-SNOM spectroscopy for yielding an accurate diagnostic test for oesophageal and other types of cancers.

Keywords: Nanophonics; cancer diagnostics

References

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PROBING THE UNOCCUPIED BAND STRUCTURE WITH LOW-ENERGY ELECTRON MICROSCOPY

Johannes Jobst[a,b], Alexander van der Torren[a], Eugene E. Krasovskii[c,d,e], Jesse Balgley[b], Cory R. Dean[b], Rudolf M. Tromp[f,a] and Sense Jan van der Molen[a]

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[f]IBM T.J. Watson Research Center, 1101 Kitchawan Road, Yorktown Heights, USA

The properties of any material are fundamentally determined by its electronic band structure. While the occupied bands can be routinely measured, it is remarkably difficult to characterize the empty part of the band structure experimentally. We now introduce a technique to measure these bands from nanoscopic samples [1]. It relies on the dependence of the reflectivity of low-energy electrons on their incidence angle on the sample and their kinetic energy. Since this angle-resolved reflected-electron spectroscopy (ARRES) is based on state-of-the-art low-energy electrons microscopy it has a spatial resolution 10nm, which is five orders of magnitude better than other techniques. We use ARRES to study the unoccupied band structure of so-called van der Waals crystals. Those custom made materials are built up by stacking layers of two-dimensional materials, such as graphene, boron nitride, or transitionmetal dichalcogenides, on top of each other. This allows it to construct crystals with specific properties that are not available in conventional materials. We also show how this novel technique can be used to shed light on the interaction between electronic states of individual layers. This knowledge is crucial for the understanding of how to tailor the properties of Van der Waals crystals in a LEGO-like fashion.

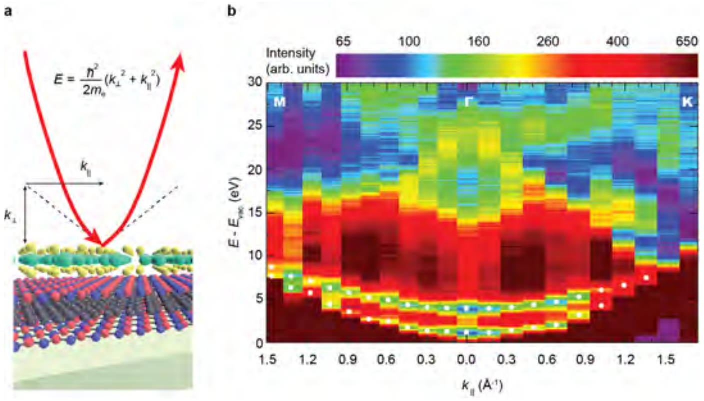

Fig. 1. **a**, Changing the angle of incidence of low-energy electrons onto a surface while recording their energy and reflected intensity yields insights into the materials unoccupied band structure. **b**, This ARRES measurement reveals, e.g., the bands of bilayer graphene and shows clear band quantization at low energies.

Keywords: Band structure; Low-energy electron microscopy; Van der Waals material

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STRUCTURE FORMATION AND ALIGNMENT OF POLYMER SEMICONDUCTORS IN THIN FILMS

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In thin films of semiconductor polymers, the polymer chains typically exhibit distinct orientation with respect to the substrate. The planar pi-face of the backbone can orient either in edge-on or face-on manner. Especially, an edge-on alignment is favorable for transport in thin film transistors, whereas face-on alignment is considered to improve vertical transport as desired in solar cells. However, molecular orientation is among the very few parameters that usually cannot be controlled when tailoring new semiconducting polymers. Here we show that both the mode of orientation as well as the degree of alignment can be well controlled by exploiting diffusive non-covalent interactions along the backbone using polydiketopyrrolopyrroles (PDPPs) as a case study.

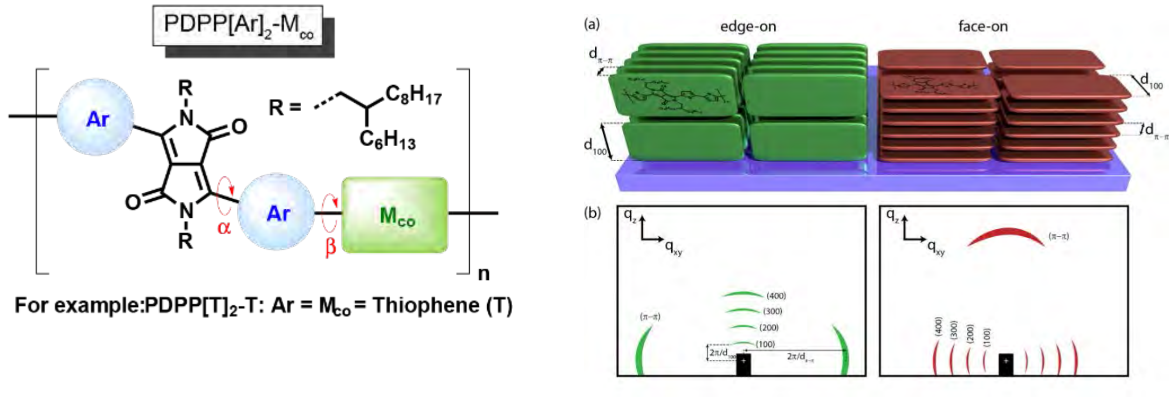

Fig.1.(left) General chemical structure of PDPPs synthesized and studied, (right) Sketch of GIWXS pattern for edge-on and face-on alignment of polymer chains

By strategically varying the chemical structure in a systematic way, we attribute for the first time, the precise control of orientation based on diffusive non-covalent interactions. Our results demonstrate how orientation in thin films of semiconducting polymers can be controlled and optimized by rational design. This study enables high-performance organic semiconductors with the additional benefit of tailored orientation that fits the desired application.

Keywords: Charge transport; Polydiketopyrrolopyrroles, molecular orientation, GIWAXS, conjugated polymers

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ELECTRONIC STATES TUNING FOR CdSe/ZnS QUANTUM DOTS UPON SELF-ASSEMBLY WITH ONLY ONE FUNCTIONAL DUE MOLECULE

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It is known that capping organic shell (including surfactants and ligands) have considerable impact on the semiconductor quantum dot (QD) surface structure and optical properties of QDs (hot carrier relaxation, quantum efficiency and photoluminescence, PL energy). Recent progress in quantum chemical calculations of structures and electronic properties of QDs has set new milestones in the understanding of QD surfaces and the capping ligand role. However, detailed and specific experimental studies on the influence of only one (or at least a few) ligand or surface attached dye molecules on surface states are difficult to conceive.

Here, we present spectral and time resolved PL data (from temperature dependent ensemble experiments) for CdSe/ZnS QD-porphyrin nanoassemblies (at molar ratio 1:1) in solvent giving rigid glassy matrix at low temperature. We have succeeded to detect the sensitivity of QD PL parameters to the chemical nature of the respective porphyrin molecules and the impact of the competing ligand layer. In addition, the results of such an elaborated investigation on an ensemble of QD-porphyrin nanoassemblies have been compared with those obtained by a newly designed and complementary (time and spectrally resolved) spectroscopy on single QDs [1]. We concluded that electronic states of different nature with varying PL energies and decay dynamic are subsequently explored on slow time scales typical for blinking phenomena which are buried but nevertheless present in ensemble experiments. Upon temperature variation the ordering of at least 2 energetically deconvoluted PL states is abruptly changed at the “phase transition”. The temperature dependence of the PL observables reveals both the influence of electron-phonon coupling between 77 K and 290 K and a “phase transition” of the capping TOPO shell at $T_{crit} \approx 220$ K. According to time resolved experiments we found at least 3 basically different types of emissive states. The specific selectivity of QD PL properties to the surface-attached only one dye molecule provides new and not yet reported experimental insights into QD surface properties. Modifications of PL properties of nanoassemblies are assigned to dye induced ligand removal accompanied by spectral blue shifts and formation of surface trap states in the band gap, and the temperature controls the energetic ordering of electronic states. The basic conclusion is that a dye molecule removes ligands from (specific) surface sites thus acting as a new “ligand” creating a modified set of new surface responsible for “Non-FRET” PL quenching upon QD-dye nanoassembly formation but not leading to FRET or charge transfer events. Such dye molecule may be considered as single molecular surface probe.

Keywords: Semiconductor quantum dots, Porphyrins, Perilene-bisimids, Ligand dynamics, Photoluminescence, Surface traps, Temperature surface “phase” transition, Blinking.

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NON-STOICHIOMETRIC Cu-In-S@ZnS NANOPARTICLES PRODUCED IN AQUEOUS SOLUTIONS BY A "GREEN" METHOD AS LIGHT HARVESTERS FOR LIQUID-JUNCTION PHOTOELECTROCHEMICAL SOLAR CELLS

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A direct "green" aqueous synthesis of mercaptoacetate-stabilized copper indium sulfide (CIS) nanoparticles (NPs) and core-shell CIS@ZnS NPs is reported. The NPs can be easily deposited onto the surface of nanocrystalline FTO/TiO_2 films yielding the visible-light-sensitive photoanodes for the liquid-junction solar cells.

Systematic variation of the NP composition, that is the content of copper, indium and sulfur, as well as the amount of ZnS deposited as a protective shell on the surface of CIS NPs showed that the highest photoelectrochemical activity was demonstrated by a TiO_2/CIS@ZnS photoanode with a molar Cu:In:S ratio of 1:5:10 and a ZnS shell produced as a molar Zn:Cu ratio of 1:1.

The photoelectrochemical activity of TiO_2/CIS@ZnS heterostructures and the photoluminescence (PL) intensity of original colloidal CIS@ZnS NPs were found to change is a similar manner at the variations of copper and indium content allowing to use PL as an indicative parameter when designing CIS-based absorbers for the solar cells. The Raman spectra of CIS NPs revealed a set of features typical for stoichiometric and copper-poorer chalcopyrite phases that is preserved after the ZnS shell formation and deposition of the CIS@ZnS NPs onto the titania surface. The X-ray photoelectron spectroscopy confirmed the copper and indium present as Cu(I) and In(III) and succesfull formation of a ZnS shell in the case of CIS@ZnS NPs.

The optimized TiO_2/CIS@ZnS photoanodes with Cu:In:S and Zn:Cu ratios of 1:5:10 and 1:1 were tested in two-electrode solar cells with aqueous polysulfide electrolyte and TiO_2/Cu_2S heterostructures produced by an original photo-assisted method as counter-electrodes. The cells revealed good stability providing steady photoelectrochemical parameters during more than 2-h continuous illumination and at least a week period of intermittent illumination as well as the excellent reproducibility of the light conversion efficiency that varied in the studied sequence of six identical solar cells not higher than by 1%. Under illumination by a xenon lamp with an intensity of 30 mW/cm^2 lamp the optimized cells showed the average light conversion efficiency of 8.2% with the average open-circuit voltage close to 0.6 V and the average fill factor of 0.42. Similar solar cells based on CIS NPs that were not covered with a ZnS shell demonstrated a far inferior activity with the light conversion efficiency around 5.8% indicating a crucial role of the passivation of surface defects of CIS NPs for achieving efficient charge collection from the TiO_2/CIS photoanodes.

The work is supported by the Volkswagen Foundation (project "New functionalities of semiconductor nanocrystals by controllable coupling to molecules").

PLASMONIC ENHANCEMENT OF RAMAN SCATTERING AND IR ABSORPTION BY QUANTUM DOTS DEPOSITED ON METAL NANOSTRUCTURES

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Metal nanostructures can lead to localised surface plasmon resonances (LSPR) with energies located in the spectral range from ultra-violet to far-infrared depending on their morphology. They can be effectively used for surface-enhanced Raman scattering (SERS) and infrared absorption (SEIRA) by semiconductor quantum dots (QDs).

Here we present the results of an investigation of SERS and SEIRA by semiconductor QDs homogeneously deposited on arrays of Au nanoclusters, dimers, and nanoantennas. The structural parameters of semiconducting and metal nanostructures were confirmed by scanning electron microscopy (SEM). The LSPR energy in the arrays of Au nanoantennas and nanoclusters as a function of their size was determined by means of IR and optical spectroscopies.

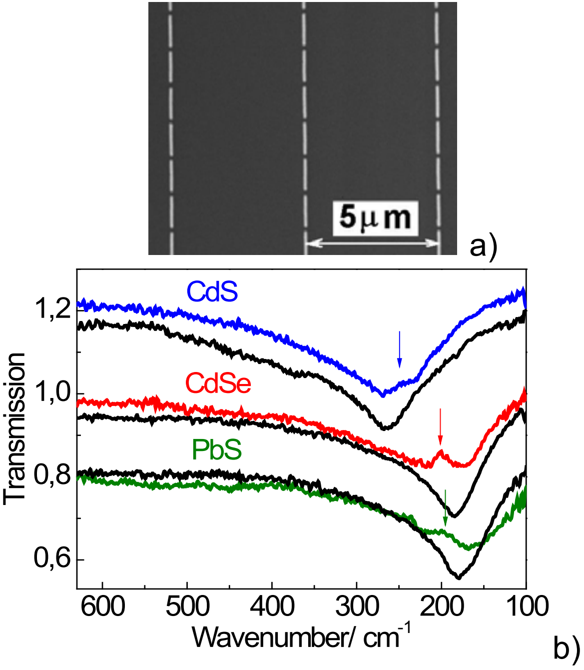

Fig.1 a)- SEM image of a Au nanoantenna array. b)- SEIRA spectra of 1 monolayer of CdS, CdSe, and PbS QDs. The IR spectra of the arrays without QDs are given for comparison.

CdSe QDs deposited on Au nanocluster arrays reveal SERS effect by confined longitudinal optical (LO) phonons in QDs. The SERS enhancement factor (EF) depends resonantly on the metal nanocluster size and thus on the LSPR energy. EF shows a polarization anisotropy for CdSe QDs on Au dimers. A confinement-induced shift of the LO phonon mode was observed for CdSe QDs deposited on the structures with single Au dimers. This shift depends on the CdSe QD size and indicates quasi-single QD Raman spectra being obtained.

3D electrodynamic simulations were used to calculate structural parameters of nanoantennas providing the maximal SEIRA enhancement at the energy of optical phonons in QDs. SEIRA by surface optical modes in monolayers of CdS, CdSe, and PbS QDs on nanoantenna arrays was observed (indicated by arrows in Fig.1b).

This work was supported by Russian Science Foundation (project 14-12-01037).

Keywords: enhancement; Raman scattering; IR absorption; phonons

Magnetic Nanostructures Designed For Hard Disk Drive Applications

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Continued progress in hard disk drive areal density for conventional perpendicular magnetic recording (PMR) based on granular media has become increasingly difficult [1]. Although adoption of energy assisted magnetic recording (EAMR), specifically Heat Assisted Magnetic Recording (HAMR) [2] is widely viewed as a promising solution for thermal stability issues, challenges in grain size scaling and managing media noise may limit the rate of progress for EAMR based on granular media. Bit patterned recording (BPR) stands as an attractive alternative to granular media, offering a path to thermally stable recording at high density and significantly reduced media noise by replacing the segregated random grains of PMR media with lithographically defined single domain islands [3,4]. Figure 1 compares and summarizes basic characteristics of currently used conventional PMR based on granular media and BPR based on pre-defined bits.

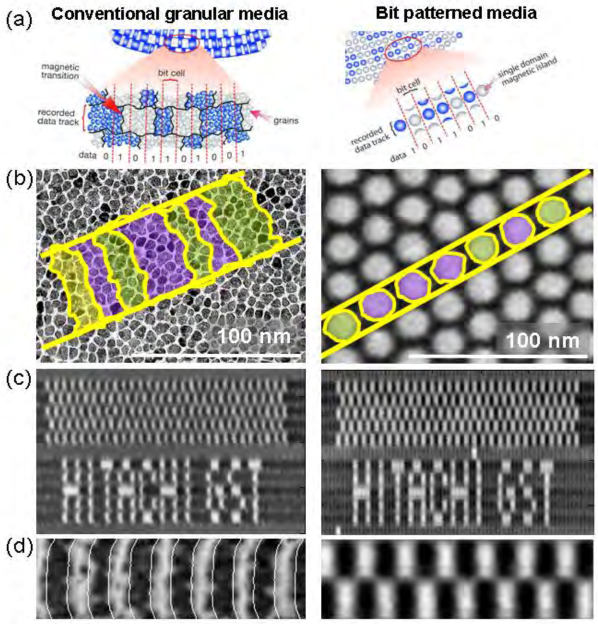

Fig. 1. Comparison of granular PMR (*left*) and BPR (*right*) media systems. (**a**) Bit scheme for both recording systems. (**b**) Bit definition within the lateral recording media microstructure. (**c**) Comparison of static read/write testing on both media systems. (**d**) High resolution images with alternating up-down bit structure for both recording systems. Bit dimensions in (**c**) and (**d**) are 145 nm cross track and 45 nm down track (~100 Gb/in^2).

In my talk I will discuss various choices for BPR magnetic materials, such as Co/Pd and Co/Pt multilayers as well as CoCrPt and FePt $L1_0$ alloys. I will highlight advantages and disadvantages of the different magnetic material systems with respect to potential applications in BPR and outline the specific challenges when comparing conventional PMR, BPR and currently emerging HAMR systems.

Keywords: magnetic recording, hard disk drive, perpendicular magnetic recording, bit patterned recording, heat assisted magnetic recording

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LONG LIFETIME OF EXCHANGE-DOMINATED SPIN WAVES IN ULTRA-THIN COBALT FILMS

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The miniaturization of magnon-based devices into the nanometer range requires the utilization of exchange-dominated spin waves with wave-length in the nm-range. Only those spin waves possess sufficiently large group velocities for a fast transport of the spin information. High group velocities are realized in particular by spin waves in ultra-thin cobalt-films. These spin waves were studied extensively in the last years using inelastic scattering of low-energy electrons [1,2]. However, because of limitations in the energy resolution the experimental data base was confined to wave vectors between about 3nm^{-1} and the boundary of the surface Brillouin zone. In that range, the lifetime of spin waves is extremely short (<100fs) [3]. Correspondingly, the mean free path of a spin wave packet (defined as the product of group velocity and lifetime) is only of the order of 1nm. For that reason the acoustic spin wave modes of 3d-metals were not considered as possible candidates for spin wave based devices.

Recent improvements in the technology of electron energy loss spectrometers now enable the studies of spin waves of wave-vectors down to 1.5nm^{-1} with an energy resolution down to 2meV [4,5]. In this presentation we report on high resolution data of those spin waves in ultra-thin fcc cobalt layers deposited on Cu(100) surfaces. The results are compared to a theory of spin excitations which takes into account the itinerant character of the electrons. For eight atom layer (8ML) films with a small density of surface steps and wave vectors q<2nm^{-1} we find lifetimes of several picoseconds, in agreement with our theory. However, those long lifetimes are observed only for well-annealed films with a small density of surface steps.

Ongoing studies on films with regular step arrays obtained by deposition on Cu(1123) and Cu(1113) substrates show that the step-induced damping is particularly severe when steps cross the path of spin waves.

Keywords: Spin waves; Cobalt films, Electron spectroscopy

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MAGNETIC MOMENTS AND HYSTERESIS OF AN ENDOHEDRAL SINGLE-MOLECULE MAGNET ON A METAL

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Endohedral fullerenes containing clusters of lanthanides are a new interesting class of molecular magnets. The magnetism of these systems depends on the number of lanthanides, their spatial arrangement and their magnetic quantum number. The magnetic hysteresis which is characteristic for single-molecule magnets, is also observed when the fullerenes are deposited on metal substrates. In my talk I will present studies on Dy-nitride cluster fullerenes. It will be shown that the interaction between the endohedral unit in the single-molecule magnet Dy2ScN@C-80 and a rhodium (111) substrate leads to alignment of the Dy 4f orbitals. The resulting orientation of the Dy2ScN plane parallel to the surface is inferred from comparison of the angular anisotropy of x-ray absorption spectra and multiplet calculations in the corresponding ligand field. Element specific magnetization curves from different coverages exhibit hysteresis at a sample temperature of 4 K. From the measured hysteresis curves, we estimate the zero field remanence lifetime during x-ray exposure of a submonolayer to be about 30 seconds.

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A microscopic view of atomic and molecular contacts: Magnetoresistance, switching, forces

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The electron transport through single atoms and molecules is investigated with low-temperature scanning probe microscopy. In the experiments, which aim at maximizing the control over the junction properties, the conductance and the acting force are probed. The talk will address the magnetoresistance of single adsorbed metal atoms and molecular switches including spin state switching.

Keywords: contact, single molecule, single atom, magnetoresistance, atomic force microscopy, spin crossover, Kondo effect

COLLECTIVE ELECTRONIC EXCITATIONS IN THIN FILMS

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Collective electronic excitations at metal surfaces are well known to play a key role in numerous phenomena, ranging from physics and material science to biology and medicine. From the fifties it is known [1] that at the planar vacuum/metal boundary a mode, called surface plasmon, emerges with frequency $\omega_{sp} = \omega_p / \sqrt{2}$, where ω_p is the bulk plasmon frequency. This relation between the bulk and surface plasmon frequencies is a manifestation of the fact that in a long-wavelength limit both quantities are entirely determined by the bulk dielectric function properties. In particular, the surface plasmon properties at small momentum transfers can be studied on base of a surface response function g [2] related to bulk dielectric function ε as $g = (\varepsilon - 1)/(\varepsilon + 1)$. In thin films, due to the presence of two surfaces, the interaction of corresponding surface plasmons produces its hybridization [1]. As a result, the dispersion of two symmetric and antisymmetric surface modes of a film with thickness L is expressed as $\omega_{sp}^{\pm} = \omega_{sp}\sqrt{1 \pm e^{Lq}}$, where q is an in-plane momentum.

In real metallic systems the dielectric function is often very different from the predictions of the free-electron-gas mode. In particular, recently it was demonstrated that indeed in many materials, like normal [3], charge-density-wave [4,5] and superconducting [6-10] metals and intercalated graphite [11], additionally to the conventional bulk plasmon, there exists a number of other bulk collective modes characterized by significantly lower frequencies. In this contribution we analyze which impact the presence of such low-energy modes in the bulk may produce on collective electronic excitations in thin films.

Keywords: Thin films; Surface plasmon; Dielectric function

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MAGNETISM AND HALL EFFECTS IN THIN FILMS OF TOPOLOGICAL INSULATORS

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Topological insulators (TIs) are narrow–gap semiconductors characterized by Dirac-like surface state and protected by time-reversal symmetry. Magnetic field (external or internal) breaks this symmetry and causes splitting of the topological surface state at the Dirac point thus making the surface insulating.
Internal magnetic field in TIs can be create in various ways, in particular, by introducing vacancies or carbon atoms [1], doping with 3d-transition metal atoms [2], displaying magnetic semiconductors or organic overlayers as well as bulk materials on the surface of three- or two-dimensional TIs [3-5].

Here we present and discuss recent results of the study of magnetic impurities as well as magnetic proximity effects on electronic and spin structure of TIs and splitting of the topological surface state. We propose a method for engineering of heterostructures that result systematically in big splitting of the Dirac cone. We also analyze magnetic effects in two-dimensional topological insulators and heterostructures and discuss recent results for quantum spin and anomalous Hall effects [6,7].

Keywords: Topological insulators; Dirac surface states; ferromagnetism; Hall effects

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PHOTONS, ELECTRONS, AND PHONONS AT THE NANOSCALE WITH TIP-ENHANCED RAMAN SPECTROSCOPY AND PHOTOTHERMAL IMAGING

Raul D. Rodriguez[a], **Adarsh Reddy**[a], **Rayhan Rasel**[a], **Zoheb Khan**[a], **Teresa I. Madeira**[b], **Harsha Shah**[a], **Eugene Bortchagovsky**[c], **and Dietrich R.T. Zahn**[a]

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The diffraction limit of light was regarded as a fundamental unbreakable barrier that prevented the visualization of objects with size smaller than half the light wavelength, until super resolution optical methods and near-field optics allowed overcoming that constraint [1,2]. We report on a new approach based on tracking the photo-thermal expansion (nano-vis) in combination with tip-enhanced Raman spectroscopy (TERS). A commercial TERS system based on atomic force microscopy is coupled to a mechanical switch for intermittent visible light excitation. This simple configuration allows detecting small changes in the nano-object volume. Contrary to nano-IR that is based on the detection of molecular and lattice vibrations [3], the principle behind nano-vis involves tracking the heat generated from electronic transitions and scattering during the relaxation in the sample material that occurs due to optical absorption in the visible spectral range. The sensitivity and spatial resolution are further improved by the combined effect of electric field enhancement obtained by excitation of localized surface plasmons, and the synchronization of mechanical resonance of the tip-cantilever system with the intermittent light excitation. Our concept is demonstrated by the TERS and nano-vis analysis of a two-dimensional material (GaSe) on graphite and by an array of multi-walled carbon nanotubes lithographically designed in a silicon oxide matrix. In addition to TERS, an unprecedented spatial resolution for optical absorption below 10 nm is reported.

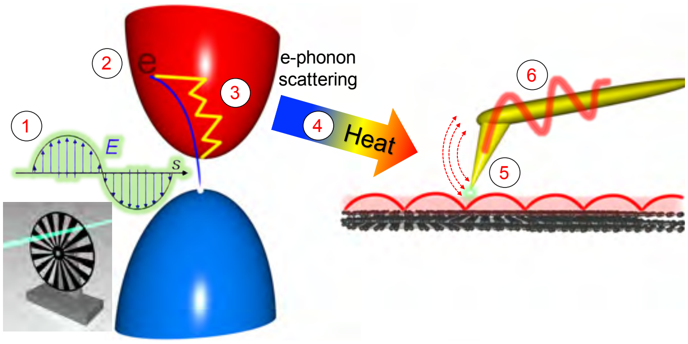

Figure 1: (a) Physical schematics behind nano-vis: (1) a chopper allows the intermittent passage of photons with energy high enough to excite an electron from the valence band to a high energy level (2) in the conduction band, non-radiative relaxation (3) mediated by e-phonon scattering induces (4) heat increase that results in the thermal expansion of the sample (5) and the cantilever deflection (6).

Keywords: nano-optics, photo-thermal imaging, tip-enhanced Raman spectroscopy, TERS, plasmonics, atomic force microscopy, optical absorption

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PHONON EFFECTS IN PLASMONIC SPECTRA

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Germany

Plasmonic resonances of metallic nanowires in the infrared are well known to be beneficial for vibrational sensing of molecules. They are also very sensitive to phononic excitations, which in case of strong coupling to phonon-polaritons leads to qualitatively different spectral behaviour. What has been considered only seldom is the influence of the metal phonons on the plasmonic resonance. In the infrared, the measurement of plasmonic resonances allows to obtain valuable quantitative information on the conductivity of the wires.[1] For example, our study of the temperature dependent plasmonic resonance spectrum of nanowires with a high crystalline quality revealed a phononic damping of the electronic excitation that with temperature increases, the stronger the thinner the wires.

Keywords: Infrared plasmonics; electronic damping; phonons; nanostructures

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Field enhancement at silicon-oxide interface layers generated by Au island films

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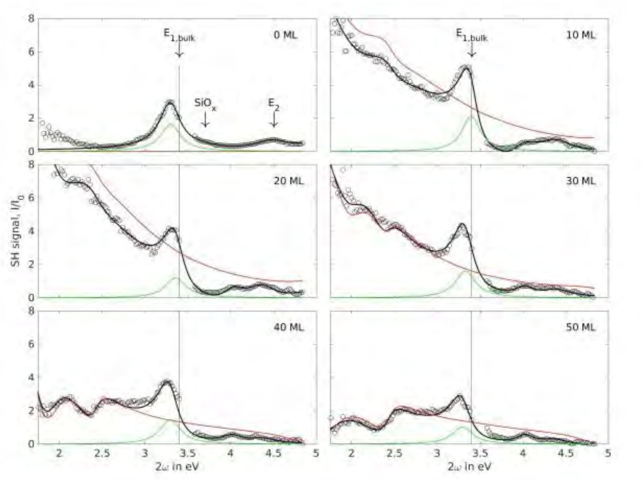
A promising applications of nanoplasmonics is the design of metallic structures that enhanced light absorption in thin film solar cells [1] where the active layer has poor light absorption. In this work field enhancements from Au ellipsoids with diameters from 30 to 250 nm deposited on a Si substrate with a thin 1 nm thick surface oxide have been investigated by second harmonic generation spectroscopy. *The basic idea of this work is to follow the relatively sharp SHG resonance from Si near the E_1 critical point in order to deduce the field enhancement inside a thin Si interface layer.*

The measured linear optical properties are well described by the island film model [2] and are used in the investigation of the SHG signal.



At energies below the E_1 critical point energy a strong SHG signal originating from plasmon resonances in the Au particles is observed. By following the evolution of the characteristic Si SHG-resonance it is found that the Au particles affect the Si SHG signal in two ways: 1) charge transfer from the substrate to the metal modifies the band bending in Si and gives rise to E-field induced SHG (EFISH) and 2) local enhancement of the field at the Si-oxide interface. For small particles the EFISH part dominates while for larger particles the field enhancement at the Si-oxide interface dominates the SH signal and a field enhancement factor in Si of 4 is found experimentally. This is about a factor of 5 less than the corresponding factor calculated by the local field factors when the separation between Au islands and the Si interface region is neglected. It is suggested that the fast decay of the local field away from the metal islands reduces the observed field enhancement.

Keywords: Plasmonics; Field enhancements; Nonlinear optics

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Improved *ab initio* calculation of surface second-harmonic generation from Si(111)(1×1):H

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CANCELED

INTERACTION OF SURFACE AND LOCALIZED PLASMONS PROBED BY ELLIPSOMETRY

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Interaction of two resonances results in their hybridization and splitting what produces the energy gap between two hybridized dispersion curves instead of their intersection. We investigated the interaction of surface plasmon with localized resonances of nanoparticles deposited on the surface.

Ellipsometry in the Krechman geometry was performed for such structures. Ellipsometry was chosen as the relevant method for the registration of surface plasmon [1] and interparticle interactions [3]. Some results are shown in Figs.1-2.

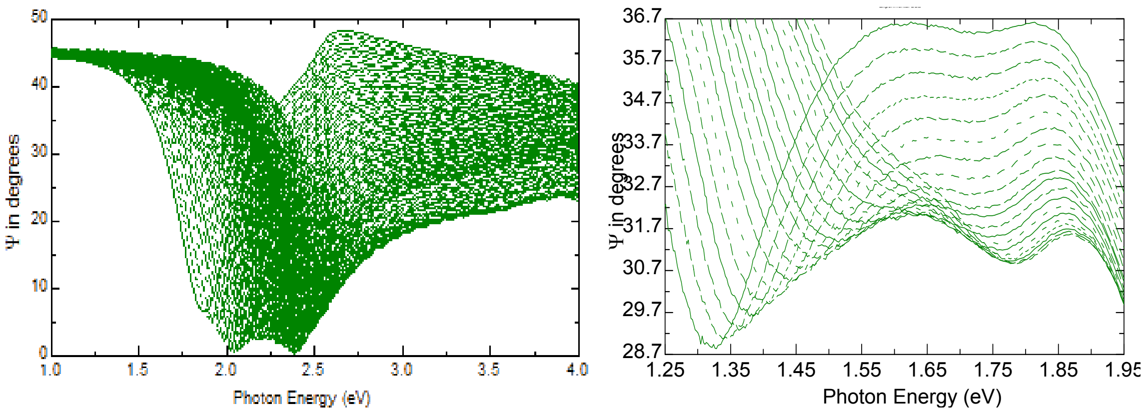

Fig.1. Spectral behaviour of ellipsometric angle Ψ for the system with deposited nanoparticles measured at internal reflection with the excitation of surface plasmon at different angles of incidence.

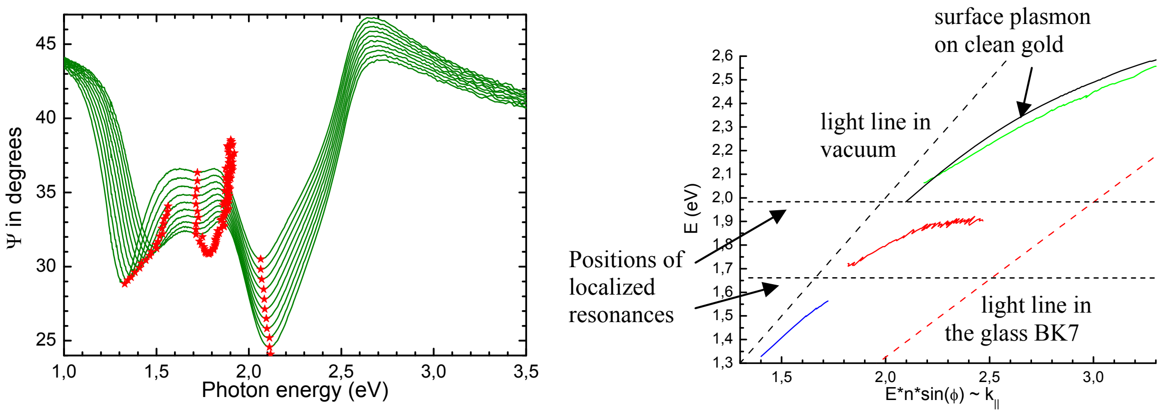

Fig.2. Position of minima of the spectra of Ψ and resulted dispersion curves.

Keywords: ellipsometry, surface plasmon, localized plasmon, splitting

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APPLICATIONS OF IMAGING ELLIPSOMETRY AND BREWSTER ANGLE MICROSCOPY IN BIO-FUNCTIONALIZATION AND SENSING – AN OVERVIEW

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A homogenous functionalization of equivalent surfaces and an accurate patterning of arrays is the desired case in bio functionalization and sensing, but the experimental reality is often different. Uncoated areas are frequently contaminated with remnants from coating of different treated sample areas (Fig. 1) or with additives of the coating process. The doughnut effect and similar issues can occur in case of drying. In some cases particles are formed by aggregation or by competitive reactions to the grafting as is frequently the case for silanization with trifunctional silanes. From the point of view of biomolecular interactions, model membranes like supported bilayers are of increasing interest. In case of mixed lipid layers, phase transition can take place forming rich and pure domains. In this case an overall averaging method is misleading. Perhaps the initialization of biofouling can be considered as a localized bio functionalization.

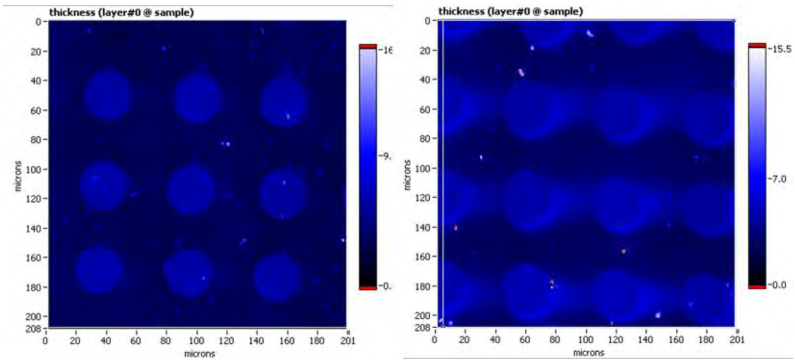

Fig. 1. Protein array on Si-wafer after washing, measured at 658 nm (laser)

The mentioned scientific questions require very sensitive, label free detection methods with a microscopic lateral resolution. The contributed paper will give an overview how Imaging Ellipsometer, Brewster Angle Microscopy and imaging Surface Plasmon Resonance Enhanced Ellipsometry (i-SPREE) can contribute in solving these questions.

Keywords: Imaging ellipsometry, Brewster angle microscopy, i-SPREE, LB-films, supported bilayers, biomolecular interaction

Tuesday:

	N112		
09:00	*Plenary Talk*: T. S. Rahman		
	N112		N113
09:45	*Invited Talk*: S. Kera	09:45	*Invited Talk*: J. S. Speck
10:45	N. Esser	10:45	J. F. Woitok
11:00	R. Schlesinger	11:00	B. Borkenhagen
11:15	S. Sakurai	11:15	U. Rossow
11:30	P. Amsalem	11:30	E. Pincik
11:45	D. A. Evans	11:45	~~N. Tolk~~
13:30	*Invited Talk*: S. Kowarik	13:30	*Invited Talk*: M. Wuttig
14:00	B. Höffling	14:00	Yu. M. Azhniuk
14:15	M. Reutzel	14:15	P. H. Thiesen
14:30	T. L. Einstein	14:30	*Invited Talk*: R. Calarco
14:45	K. Bobrov		
15:30	M. Scheele	15:30	*Invited Talk*: S. Murakami
15:45	*Invited Talk*: M. Grundmann		
		16:00	C. M. Acosta
16:15	I. Arnay	16:15	~~K. Schouteden~~
16:30	P. S. N. Barimar	16:30	*Invited Talk*: A. Kimura
16:45	C. Schmidt		
17:00	Poster session		

TAILORING CHEMICAL AND OPTICAL PROPERTIES OF 2D TRANSITION METAL DICHALCOGENIDES

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Single-layer of molybdenum disulfide (MoS_2) and other transition metal dichalcogenides (TMDC) appear to be promising materials for next generation applications (optoelectronic and catalysis), because of their low-dimensionality and intrinsic direct band-gap which typically lies in the visible spectrum. Several experimental groups have already reported novel electronic and transport properties which place these materials beyond graphene for device applications. MoS_2 is also known to be a leading hydrodesulfurization catalyst. Efforts are underway to further tune these optoelectronic and catalytic properties through alloying, defects, doping, coupling to a substrate, and formation of bilayer stacks (homo- and hetero-structures). In this talk I will present results from joint theoretical and experimental investigations [1-3] which provide a framework for manipulating the functionality of this wundermaterial and take us closer to the goal of rational material design. With emphasis on the chemical properties of defect-laden single layer MoS_2, I will examine modulations in its local atomic environment (see Fig. 1 for an example) under which it could serve as a catalyst for the conversion of synthetic gas (CO and hydrogen) to methanol. With regard to the optical properties, I will present results of our analysis of the excitation spectrum and the ultrafast charge dynamics in both single- and bi-layer TMDCs obtained through the application of combined time-dependent density functional theory and many-body theory approach. In particular, I will show how the reduced electron screening in these systems leads to surprising large binding energy of electronic bound states [4] - excitons (hundreds of meVs), trions (tens of meVs) and biexcitons, in rather good agreement with available experimental data. I will also show that ultrafast (10-100fs) transfer processes are possible in these materials as a result of strongly-delocalized hole orbitals. Possible technological applications will be discussed.

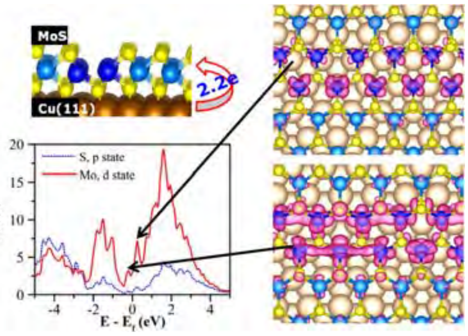

Fig. 1. Single layer MoS_2 grown on Cu(111)

Single-layer molydenum disulfide*:* transition metal dichalcogenide; exciton; catalysis

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A PERSPECTIVE OF QUASIPARTICLE STATE IN ORGANIC CRYSTALS

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Understanding the impacts of strong electron-phonon coupling as well as weak electronic interaction on the electronic state is required to discuss the rich of functionality in organic molecular materials. Angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) is known to be a powerful technique to study the electronic states. However, the experimental study of fine features in the highest occupied molecular orbital (HOMO) state has not been progressed till recently due to difficulty in the sample preparation, damages upon irradiation and so on, though it can offer a wide variety of key information, that is essential to comprehend charge-hopping transport and small-polaron related transport in the ordered monolayer film [1] as well as to coherent band transport in the molecular single crystal [2,3]. We present recent findings regarding on the precise measurements of electronic states for large aromatic organic molecular materials by using high-resolution ARUPS. A quasiparticle state is appeared differently in the UPS spectrum depending on the strength of the intermolecular interaction which is confirmed by the width of the energy band.

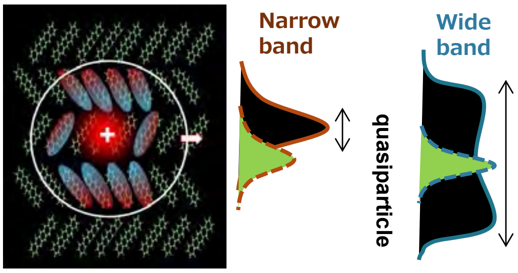

Fig. 1. HOMO-band features found as a polaron formation in organic crystals

Keywords: rubrene, electron-phonon coupling, small polaron, photoelectron spectroscopy

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SURFACE RESONANT RAMAN SCATTERING FROM THE BARE AND THE (2x1)-O-RECONSTRUCTED Cu(110) SURFACE

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In recent years Raman spectroscopy has been successfully employed to study surface vibrational modes of semiconductors via surface resonant Raman scattering. Metals like Cu, Ag, Au, on the other hand, which are important substrates for Surface Enhanced Raman scattering from rough surfaces, are not expected to show Raman signals, due to their crystal structure. As it is known from inelastic electron and He atom scattering the highly anisotropic Cu(110) surface exhibits a characteristic set of vibrational modes. Therefore, it is of particular interest that our surface Raman experiments show that the symmetry breaking on the metal surface enables indeed inelastic light scattering from surface phonon modes. This makes possible new high spectral resolution measurements of the same set of surface vibrational modes and a determination of their intrinsic lifetimes. Comparison of polarization resolved measurements with calculations of the surface vibrational modes provides indications to the enhancement mechanism responsible for the pronounced Raman scattering cross sections and the differences to particle scattering. Oxygen adsorption and the (2x1)O reconstruction of the Cu(110) surface gives rise to a distinct set of surface vibrational modes observable in Raman experiments. The coupling between the Cu(110) surface and the Cu-O chains in the topmost layer can be further clarified by comparison to detailed calculations.

Keywords: Surface Raman Spectroscopy, surface phonons, surface structure

Energy Level Control at ZnO/Organic Semiconductor Interfaces

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Hybrid inorganic organic systems (HIOS) are promising candidates for future (opto-)electronic devices by taking advantage of the complementary beneficial properties of two different material classes. However, inadequate interfacial energy level alignment is an intrinsic obstacle to superior device function. Hence, to design efficient HIOS devices, understanding and controlling HIOS energy level alignment is a key factor. Employing molecular electron donor or acceptor interlayers to tune the work function (ϕ) of a metal and thus the energy level alignment relative to an organic semiconductor (OSC) was reported previously [1].

In this contribution the concept is extended to HIOS interfaces comprising ZnO. The ϕ and energy level alignment modification caused by deposition of several donor and acceptor molecules onto different ZnO faces is investigated. ϕ reductions down to 2.2 eV by using the organometallic donor $[RuCp^*mes]_2$ [2] and ϕ increases up to 6.4 eV using perfluorinated tetracyanoquinodimethane (F4TCNQ) [3] are demonstrated. For molecular acceptor adsorption, significant adsorption induced upward band bending of up to 0.9 eV is found within ZnO, whereas for donor adsorption no downward bending could be induced. Exploiting the huge ϕ modifications of ZnO, upward and downward HIOS energy level readjustments are shown, which realize ultimately low electron- or hole-injection barriers at the HIOS interface. Moreover, by using an OSC whose gap matches that of ZnO, the energy level offsets at the HIOS interface could be eliminated. This enables highly efficient, non-quenched energy transfer across the HIOS interface, which is usually inhibited by unfavorable energy level alignment.

Keywords: ZnO, energy level alignment, energy transfer

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Investigation of electronic structure at cathode interfaces in Sub-phthalocyanine acceptor based organic solar cells

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Subphthalocyanine (SubPc) acceptor based organic solar cells (OSCs) exhibited superior device efficiency of over 8% [1]. However, the energy loss at the cathode/organic hetero-interfaces, e.g., formation of energy barrier, has not been clarified yet. In this study, we investigated the electronic structures at SubPc/buffer/Ag heterointerfaces by means of synchrotron based ultraviolet photoelectron spectroscopy (UPS).

The SubPc/buffer/Ag heterostructures were formed by depositing buffer materials on Ag and subsequently depositing SubPc onto buffer/Ag stack structure in a step-by-step way in a vacuum deposition chamber. A series of pyridine based acceptor molecules (BCP, TPBi and TAZ) were applied as the buffer layers.

For all buffer/Ag stack structures, metal induced gap states within the HOMO-LUMO gap were observed. These states were located near the LUMO levels and their density of states reached to the Fermi level. Thus, the gap states act as shallow donors, which enhance the electron conductivity of the buffer layers. Since the work function of the buffer/Ag stack structures showed fairly small values (3.3-3.5 eV), which corresponds to the electron affinity of the SubPc layers (~3.3 eV), the buffer layers have a role of promoting a smooth carrier injection from cathodes to acceptor layers. Nevertheless, the energy difference between LUMO of SubPc and Fermi level of buffer is estimated to be ~0.6 eV. The carrier injection barrier of the system was quite huge as compared with that of C_{60}/buffer/Ag heterostructure (~0.2 eV). The difference in the barrier height might be caused by the density of disorder originated tail states in the acceptor layers and/or acceptor/buffer heterointerfaces [2] since structural disordering is easily introduced in non-planar aromatic systems (SubPc). We consider the disorder originated tail states, which were located at the deep energy position, caused the carrier injection barrier at the SubPc/buffer/Ag heterostructures.

Keywords: energy level alignment; organic solar cells; ultraviolet photoemission spectroscopy

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THE ENERGY LEVELS IN HOLE-DOPED MOLECULAR SEMICONDUCTORS

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Understanding the nature of charge carriers in organic thin films is crucial in order to achieve rational design in opto-electronic organic devices. In the present work, we rely on interface doping phenomena, as occurring when contacting an organic semiconductor with a high work function (modified) electrode, to study the electronic properties of a hole-doped molecular thin film [1,2]. The investigated system, consisting of a C_{60} film adsorbed Au(111) pre-covered with a thin MoO_3 layer, is studied by direct and inverse photoemission. A detailed analysis of the photoemission spectra, supported by theoretical calculations based on density functional theory, helps to precisely identify the corresponding density of states of the neutral and positively charged C_{60} coexisting at the surface.

The obtained results reveal a picture of the electronic structure which strongly differs from the traditionally conceived one, i.e. with the energy levels consisting of singly occupied molecular states lying within the energy gap of the semiconductor (Fig. 1. a) [3]. Instead, here we demonstrate that the on-site Coulomb repulsion splits the partially unoccupied frontier molecular level in the p-doped systems into two sub-levels (Fig. 1. b) [1]. The role of inter-site Coulomb interaction between molecular ions and neighbor molecules is further addressed and allows providing a complete picture of the energy levels of molecular semiconductors in the presence of excess charges [1].

Keywords: Organic semiconductors; photoemission; electronic structure; hole-doping

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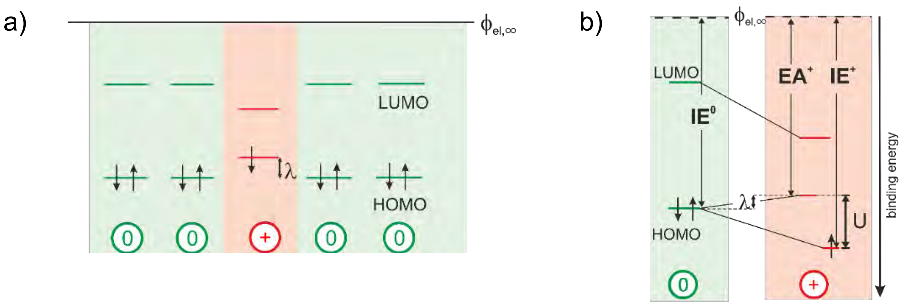

Fig. 1. a) Traditionally envisioned energy levels of positive polarons (red) embedded in a neutral organic matrix (green). b) Effect of the on-site Coulomb repulsion on the frontier energy levels upon hole doping as determined by (inverse) photoemisson.

Adsorption of organic molecules on transparent semiconducting substrates.

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The adsorption of organic molecules on semiconducting substrates is relevant to many applications from energy generation to drug delivery. Surface analysis using combined methods provides the most complete picture of surface structure, chemistry and electronic states, especially when a combination of methods is applied in-situ and in real time.

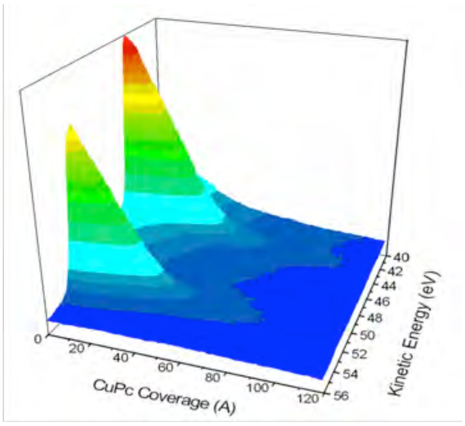

Fig. 1. Real-time monitoring of the growth of a CuPc film on a transparent oxide substrate.

Transparent oxides such as indium tin oxide (ITO) are almost exclusively used as substrates in photovoltaic (PV) devices for solar energy, usually as thin films on glass substrates. However, there is a growing interest in alternative and specialist substrates, for example UV absorbing materials for organic PV (e.g. ZnO) and ionizing radiation resistant substrates (e.g. diamond).

We have applied in-situ surface analysis to the growth of small organic molecules on several substrates to optimize the substrate, the thin film growth and the interface energetics[1]. Rapid screening and improved accuracy is achieved by data collection in real time as shown in Fig. 1 for CuPc growth on an ITO substrate. The attenuation of the substrate core level peaks provides the thin film growth mode (layer-by-layer in this case) while the energy position quantifies changes in band-bending and surface conductivity. Lineshape analysis reveals chemical changes and the optical gap of the organic semiconductor[2]. The complete interface energetics are provided by the excitation of core and bonding electrons using a range of sources from optical to UV to x-ray. For ZnO, this approach has enabled the high work function and 2-d conduction of the (0001) surface to be preserved at the inorganic-organic interface.

Keywords: Interfaces; Organic semiconductors; photovoltaics

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PURE AND DISORDERED GROUP III NITRIDE HETEROSTRUCTURES: GROWTH AND PHYSICAL PROPERTIES

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MBE growth of GaN and its alloys has advanced to the level where its is now the technique that has demonstrated the highest quality group III nitride layers and heterostructures. In this presentation we review our work on three main topics: (i) the realization of high electron mobility and high hole mobility bulk GaN by NH_3 MBE [1]. The work on p-GaN demonstrates the importance of *reduced* growth temperature to avoid natural compensation by native donors [2]. (ii) For lateral electron devices, we demonstrate the realization of pure AlN interlayers (via atom probe tomography) by plasma-assisted MBE for AlGaN/AlN/GaN and InAlN/AlN/GaN high electron mobility transistors [3]. The pure AlN interlayer allows the realization of record low sheet resistance 2DEGs. (iii) We demonstrate the surprising role that natural alloy fluctuations play in the vertical transport through nominal alloy heterobarriers [4,5]. In all of these studies, MBE has played an essential role in understanding the physical properties of the group III nitrides.

Keywords: MBE; Gallium Nitride; Transport

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TOWARDS AUTOMATED ANALYSIS OF X-RAY RECIPROCAL SPACE MAPS FOR THE CHARACTERIZATION OF GAN BASED HETEROSTRUCTURES

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Research efforts continue on the development of GaN based band gap engineered materials which find applications in HEMTs or LEDs. These devices contain epitaxial layered structures of increasing complexity. X-ray diffraction is one of the basic analytical methods that is routinely utilized for both materials research and quality control in production. X-ray scattering methods are non-destructive and deliver very detailed structural information on epitaxial layers and substrates including strain, strain relief, film thicknesses, crystalline quality and mosaic spread.

Maps around reciprocal lattice spots (RSM) can reveal additional information beyond that provided by single line scans such as high-resolution rocking curves. RSMs are typically used to aid the interpretation of peak displacement, peak broadening or peak overlap. However, they are considered too time consuming to collect and therefore are not frequently used.

Recent advances in X-ray area detector technology combined with smart positioning algorithms and data processing allow now RSMs to be recorded in similar timescales as rocking curves. These high-speed measurements find applications in the characterization in all crystalline advanced materials. Position sensitive detectors allow collecting many points at once and can be used in continuous mode, so less measurement and positioning steps are necessary to build up a given area of reciprocal space.

This contribution will discuss opportunities and limitations of this technique in conjunction with a feasibility study about automatic evaluation of RSM data from GaN based heterostructures. A fully automated workflow enables new possibilities of X-ray metrology in even high-throughput production environments.

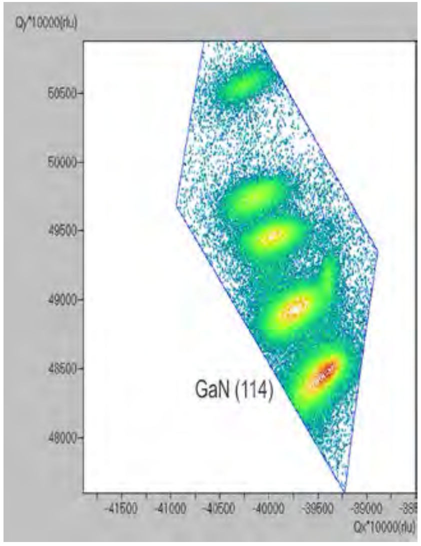

Fig. 1 **Ultra-fast RSM collected in 30 seconds on a AlGaN/ GaN HEMT structure on Si (111)**

Keywords: High-resolution X-ray diffraction; Reciprocal space map; GaN

TAILORING SINGLE-DOMAIN Si(100) SUBSTRATES FOR GaP GROWTH BY Ga-DRIVEN TRANSFORMATIONS OF SURFACE STEPS AND TERRACES

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For GaP-on-Si(100) heteroepitaxy, currently considered as a model system for monolithic integration of III-V semiconductors on Si(100), the surface steps of Si(100) have a major impact on the quality of the GaP film. Monoatomic steps cause antiphase domains in GaP with detrimental electrical properties. A viable route is to grow the III-V epilayer on single-domain Si(100) with biatomic steps, but preferably not at the expense of reduced terrace widths introduced by miscut substrates.

We have performed in situ investigations of the influence of Ga deposition on the surface terrace kinetics of Si(100) at elevated substrate temperatures by low-energy electron microscopy (LEEM). Starting from nearly equally distributed T_A- and T_B-terraces of a two-domain Si(100) surface, submonolayer deposition of Ga resulted in a transformation into a surface with prevailing T_A-terraces (Figure 1). By increasing deposition rate or decreasing temperature, we induced restructuring of Si(100) into a surface dominated by T_B-terraces as previously reported by Hara et al. [1]. The occurrence and mutual transformations of surface structures with different terrace and step structures in a narrow range of temperatures and Ga deposition rates are discussed (Figure 2).

The evolution of these surface structure transformations proceeds via three stages: (i) fluctuations of vicinal monoatomic steps, (ii) local merging of adjacent fluctuating steps and formation of a local biatomic step acting as nuclei for (iii) biatomic step growth along the direction of the steps (Figure 3).

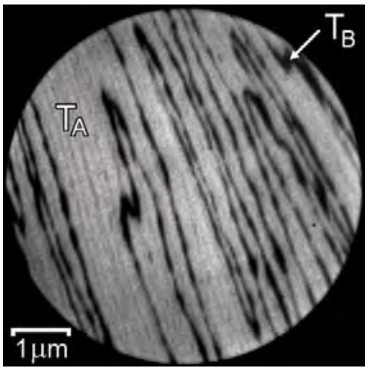

Figure 1. Dark-field LEEM image of a 90:10 distribution of T_A and T_B terraces on well-oriented Si(100) after 40 minutes of Ga exposure at 660 °C.

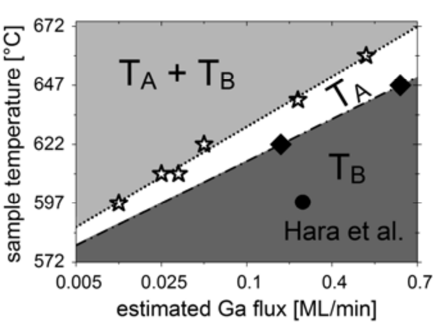

Figure 2. Existence regions for domain structures of Si(100) as a function of temperature and Ga flux. Stars and diamonds denote parameters for transformations into T_A- and T_B-dominance, respectively.

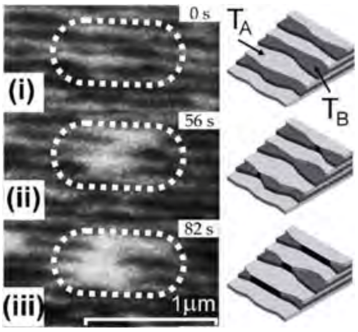

Figure 3. Ga-driven formation of biatomic steps and a local T_A domain.

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Surface processes during InGaN quantum well growth

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The active region of optoelectronic devices in the visible range based on group-III-nitrides is conventionally built from InGaN/GaN quantum well (QW) structures. For the performance of such devices control over the indium incorporation is mandatory. For long wavelengths emitters or solar cells layers with high indium concentrations ($x_{In} > 0.2$) are required. The more indium is to be incorporated the more such layers suffer from various effects such as high strain, defect formation and poor surface morphology as a consequence of the required low growth temperatures T_G. While at high T_G and lower values of $x_{In} < 0.2$ indium incorporation is limited by desorption, the growth process at lower temperatures is much more complex: Diffusion/cluster formation and desorption compete with indium incorporation. However, at least at low T_G indium incorporation takes place from a liquid-like adlayer [1,2]. The detailed structure of the adlayer and details of the interplay between indium incorporation - adlayer and adlayer formation - desorption are not yet understood.

To gain more insight into the indium incorporation process and the role as well as the properties of the adlayer we performed in-situ optical reflectivity experiments during MOCVD growth. Growth took place in a commercial Aixtron Aix200rf system with horizontal reactor using standard precursors. The system is equipped with a Laytec optical sensor which provides data on the curvature, the reflectivity at 633.2nm/950nm and the growth temperature by pyrometry.

We find evidence for indium on the surface during the time the precursor Trimethylindium (TMI) is supplied for low temperatures of about 970K (measured by a thermocouple). At these conditions the incoming flux is larger or equal to the desorption rate. The data reveal indium desorption and at least another loss mechanisms and possibly some reconfiguration of the surface (coverage). Furthermore, another source of indium is present delivering indium when TMI is already switched off.

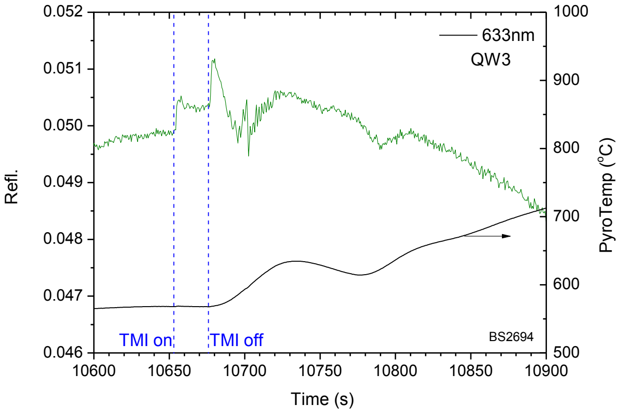

Fig. 1. Reflectivity transient taken during growth of the third QW in a 5xQW structure.

Keywords: Group-III-nitrides, reflectivity transient, adlayer

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BLACK SILICON AND ITS APPLICATION IN SOLAR CELLS

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CANCELED

Solar cell structure need low reflectance surface to maximize number of absorbed incident photons. Usually antireflection (AR) coatings are used in the solar cell industry. Their utilization is limited because they reduce reflection for narrow range of the light wavelengths. Jansen et al. [1] firstly demonstrated replacement of conventional AR coating by black silicon layer. Nanocrystalline [illegible] Si is formed by electrochemical reaction utilizing catalytic mesh. The [illegible]ical solution penetrates through the space region of the nanocrystalli[illegible]sequently, the nanocrystalline Si layer grows. In this co[illegible]sent i) photoluminescence (PL) properties of black silico[illegible]mples (without RCA treatment) measured at 6K and [illegible]r cell structures prepared on two black silicon sa[illegible]d on the BS sample with overlayer thickness of a[illegible] reference samples. All samples were prepared o[illegible] samples with following different thickness of BS o[illegible] production of the corresponding solar cells: ~ 60 [illegible] the photon energy region 1.3 eV – 2.5 eV [illegible] were not received on [illegible] reference sample after [illegible] RCA cleaning. On t[illegible] other side refe[illegible] sample after [illegible] procedures [illegible] generated [illegible] the ab[illegible] photon[illegible] Figure [illegible] signal of th[illegible] sample and [illegible] polished c-Si [illegible] recorded at ~ 6K in photon energy region 1.3 eV – 2.5 eV.

Keywords: Black silicon, Photoluminescence, Solar cell

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DEPTH-DEPENDENT STUDIES OF ELECTRON AND PHONON ULTRAFAST DYNAMICS IN FEMTOSECOND LASER INDUCED TRANSIENT STATES OF MATTER

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CANCELED

Ultra-fast laser pump-probe interactions with dielectric materials far from equilibrium provide a unique approach to both characterize and non-thermally modify these material systems [1, 2]. For example, short-pulse laser induced coherent acoustic phonons (CAP) provide a moving surface, indeed a moving mirror, which, when used in a simple reflection probe mode, has been shown to reveal strain, defect concentrations, and impurity concentrations as a function of depth with unparalleled sensitivity and depth resolution [3, 4]. This has opened exciting new avenues of exploration in the fields of nanoscale materials characterization and manipulation. To extend this approach, the realization that the CAP wave does indeed constitute an actual [illegible] surface, suggests that surface physics techniques that have been routinely ap[illegible]aracterize normal surfaces and interfaces may be applied to the moving CAP [illegible]

In this presentation, we will discuss ongoing resea[illegible]damentals of coherent acoustic phonon spectroscopy, (b) semico[illegible]centration profiles measured using coherent acoustic phono[illegible] ultrafast carrier and phonon dynamics of graphene on [illegible]acilitating ultrafast laser induced low-temperature [illegible]chemes for accomplishing depth dependent materials [illegible]ent states of matter.

Keywords: Coherent Acoustic Phonons; Ph[illegible] Graphene; Second Harmonic Generation

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Novel control strategies in molecular thin film deposition: from tailoring crystallinity and morphology to patterning of films

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Crystal structure and resulting electronic and optical properties of materials and thin films can increasingly be predicted by theory. However, despite advances in unraveling the mechanistic details of the thin film growth process, film properties such as morphology, grain size and defect density are rarely modelled before film deposition. To take our understanding beyond a recipe-based perspective to that of sound fundamental understanding we use real-time X-ray observation of growth processes (using growth oscillations and small angle scattering) to understand the atomic scale processes. We derive the energy barriers for diffusion and step edge crossing from X-ray data for examples of organic semiconductor thin films (C_{60} and PTCDI-C_8 molecules). Using this detailed understanding of growth processes we demonstrate different strategies to tailor film growth. We will demonstrate how fast temperature modulation instead of a constant substrate temperature can be used to tailor the nucleation phase of each successive monolayer to achieve smoother film growth. As another new control parameter in molecular film growth we show that light can be used to increase phase purity in organic thin films. We will further demonstrate how polarized light can be used for photo-alignment during molecular thin film growth by addressing specific anisotropic absorption bands, such as the lower Davydov component of tetracene films. The illumination allows us to achieve photo-alignment of the otherwise randomly oriented polycrystalline tetracene films and also enables patterning of films, e.g. for photonic meta-films or electronic applications.

ELECTRONIC PROPERTIES OF PPP@ZnO FROM ALL-ELECTRON QUASIPARTICLE CALCULATIONS

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We investigate the electronic properties of poly(*para*-phenylene) (PPP) adsorbed on the non-polar (001) surface of rocksalt (*rs*) ZnO using all-electron density functional theory (DFT) as implemented in the *exciting* code [1] as well as the *GW* method to treat quasiparticle excitations within many-body perturbation theory. A comparison of the derived electronic band offsets at the interface with various mesoscopic alignment methods, such as the Shockley-Anderson approach [2] or the alignment via the electrostatic potential [3] shows the inadequacy of these methods for molecular adsorption even for physisorbed molecules with no charge transfer at the junction.

We discuss the influence of quantum confinement, charge transfer and molecular polarization as well as the impact of electron-phonon coupling on the electronic band discontinuities and the methodological implications for the *ab-initio* description of interface electronics.

Keywords: electronic structure theory; organic-inorganic heterostructures; hybrid systems; band-level alignment

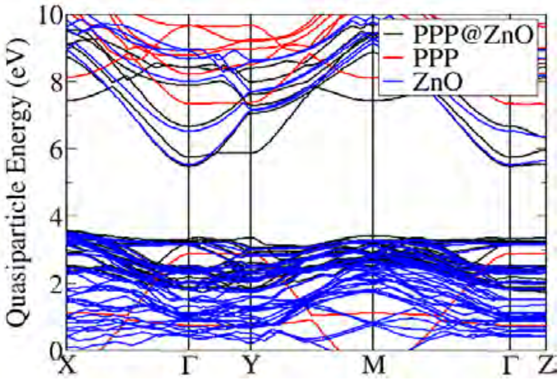

Fig. 1. QP band structure of PPP@*rs*-ZnO

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Chemoselective Reactivity of Bifunctional Cyclooctynes on Si(001)

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Organic functionalization of semiconductor surfaces and its potential for the miniaturization in semiconductor technology has motivated detailed investigations of the adsorption of organic molecules on semiconductors, especially on silicon. However, controlled organic functionalization of semiconductor substrates under well-defined vacuum conditions has not been achieved so far. The challenge is the chemoselective covalent fixation of bifunctional molecules on these substrates leaving the remaining second functional group available for further building up of complex molecular architectures. The main difficulty in achieving the required chemical selectivity on semiconductor surfaces, especially on the technologically most relevant Si(001) surface, arises from the high reactivity of their dangling bonds; typically, a mixture of molecules adsorbed with different functional groups is observed.

In this contribution, we present STM- and XPS-experiments on the adsorption configurations of bifunctional cyclooctyne derivates with different functional side groups. These molecules show indeed such a chemoselective fixation: The strained cyclooctyne triple bond adsorbs selectively on-top of a silicon dimer while leaving the other functional groups intact. The achieved chemoselectivity is explained taking the distinctly different adsorption dynamics of the separate functional groups into account: Using molecular beam techniques, we demonstrate a direct adsorption pathway for the strained cyclooctyne triple bond. This is opposed to the majority of most organic functionalities, which generally adsorb on Si(001) via a metastable intermediate state. Thus, even if the cyclooctyne derivate first adsorbs in this metastable intermediate, the reaction of the strained triple bond is still accessible and in fact kinetically more favorable than the further reaction of the other functional group.

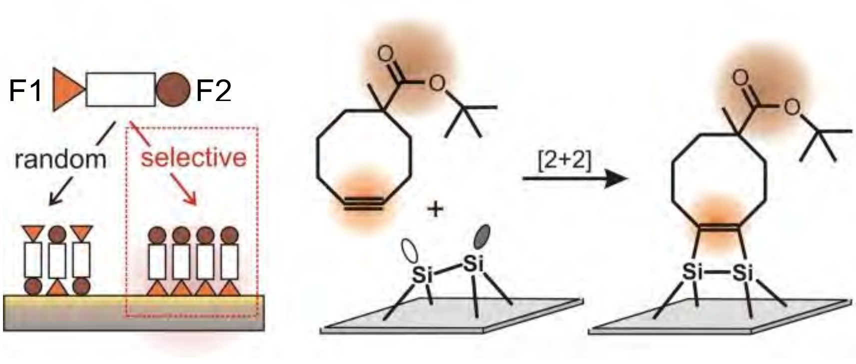

Fig. 1. (left) Schematics of the adsorption process of bifunctional (F1, F2) organic molecules on Si(001). The high reactivity of the surface dangling bonds leads typically to a random adsorption via F1 or F2. (right) In the case of bifunctional cyclooctyne derivates, a chemoselective adsorption with the strained triple bond is observed; F2 stays intact for further functionalization.

Keywords: Surface Chemistry; Surface Reactions; Reaction Dynamics; Si(001); Cyclooctyne

SUBMONOLAYER ISLAND GROWTH OF ORGANICS: CAPTURE-ZONE DISTRIBUTIONS, GROWTH EXPONENTS, & TRANSIENT MOBILITY*

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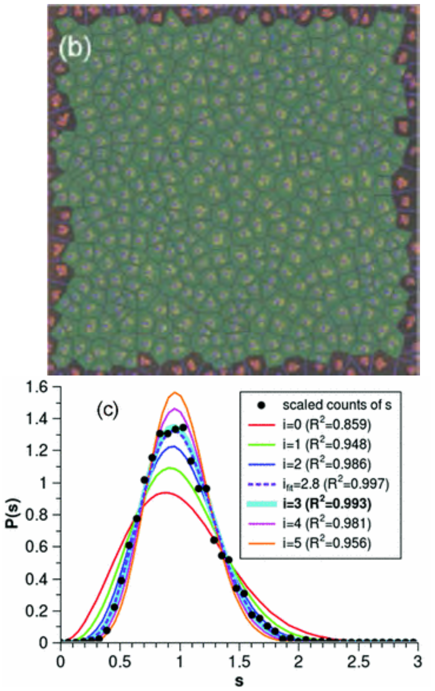
Analyzing capture-zone distributions (CZD) using the generalized Wigner distribution (GWD) has proved a powerful way to gain insight into epitaxial growth, in particular to access the critical nucleus size i, as reviewed in [1]. The CZ of an island contains all points closer to that island than to any other, a generalization of Wigner-Seitz cells known as a Voronoi tessellation. This approach complements measurements of the growth exponent α from the scaling (with flux F) of island density $N \propto F^{\alpha}$ and of the distribution of island sizes. We summarize some extensive Monte Carlo simulations and especially experiments on various systems to which the GWD has been applied, emphasizing organic adsorbates. Others include atomic (sometimes with impurities), quantum dots, and colloidal nano-particles. In the case of parahexaphenyl (6P) on sputter-modified mica [2], the value i extracted from CZD (see figures) differs from the [larger] values of i deduced from $N \propto F^{\alpha}$. Furthermore, the values of i differed considerably at small and large F, which was attributed to DLA and ALA dynamics [2]. To reconcile the CZD and scaling measurements, we took into account long-known transient mobility (hot precursors) [3]. Similar behavior is seen for pentacene adsorbates. We close with applications of the GWD to social phenomena, notably the areas of Voronoi tessellations of subway stations and of secondary administrative units (e.g. French arrondissements and German Landkreise) [4]. In some other cases (e.g. Dutch gemeenten and Turkish ilçeler) a lognormal distribution accounts better for the data. We discuss the source and note analogous behavior in surface phenomena.



b) Voronoi tessellation for islands of 6P on sputtered mica; c) analysis of distribution $P(s)$ of s, cell areas [÷ average area] using GWD [2]

Keywords: Deposition of organic molecules, growth on surfaces, size distributions

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THERMODYNAMIC BALANCE OF PERYLENE SELF-ASSEMBLY ON Ag(110)

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We present a room temperature STM study of perylene adsorption on Ag(110) at the monolayer coverage regime. We found that structure and symmetry of the flat perylene monolayer is determined by thermodynamic balance of the three factors: (i) the site recognition effect, (ii) the intermolecular interaction and (iii) the thermal motion of the perylene molecules. The moderate strength of the site recognition and intermolecular interactions, of the same order of magnitude as *kT* ~25 meV, represented a key feature of the thermodynamic balance.

The thermodynamic balance bestowed to this system the unique quality to form a flexible monolayer of epitaxial as well as self-assembling character. The increasing perylene coverage induced gradual crystallization of the initially fluid monolayer (<0.1 ML) into the crystalline (2 5 3 -2)/(2 -5 3 2) monolayer (0.1053 ML). The crystalline monolayer further incorporated extra molecules modifying its structure and symmetry albeit maintaining its true commensurate character. The recognition effect of moderate strength was able to lock some of the perylene molecules into favorable adsorption sites of the (110) lattice providing a skeleton of the crystalline phases. We have found that the crystalline monolayer did not quench thermal motion of the included molecules but rather accommodated it modifying its skeleton by reselecting a new set of available adsorption sites favorable in terms of intermolecular interaction.

The ability of the perylene crystalline structure to accommodate its thermal motion made possible formation of the epitaxial and self-assembled perylene monolayer free of domain boundaries in the whole coverage range.

Key words: perylene, Ag(110), organic monolayer, self-assembly, epitaxy, surface mobility, thermodynamics, fluid phase, STM

Thin Films of Coupled Organic-Inorganic Nanostructures

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The concept of coupled organic-inorganic nanostructures provides a new approach to electronic applications of colloidal nanocrystal (NC) superlattices for power conversion or lighting purposes. [1] A typical superlattice consists of periodically alternating NCs and monolayers of coordinating organic semiconductor (OSC) small molecules, which act as electronic coupling agents to promote charge carrier transport across the lattice of NCs. I will show how the OSC is utilized to guide the self-assembly of semiconducting or metallic nanocrystals into quasi-2D thin films which are conductive and highly ordered at the same time. [2,3] The thin films are obtained as free-floating membranes at the liquid/air interface, transferred to solid substrates and characterized in real space by high-resolution TEM, HAADF-STEM as well as in reciprocal space by GIXD, GISAXS and simultaneous SAXS/WAXS utilizing a nano-beam set-up. The optoelectronic properties inferred from electric transport measurements, optical spectroscopy and transient absorption are discussed in the light of utilizing these hybrid thin film materials for applications in LEDs, photodetectors, sensors and thermoelectrics.

Keywords: Colloidal nanoparticles; hybrid nanomaterials; Optoelectronics

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SEMICONDUCTING OXIDE THIN FILMS: NOVEL RECTIFYING CONTACTS FOR ELECTRONIC AND PHOTONIC APPLICATIONS

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We present a number of novel rectifying material combinations (thin film heterostructure diodes) involving semiconducting oxides that provide excellent rectification [1]. We discuss the interfaces and the physical mechanisms of rectification, device properties and the possible use in applications. Three diodes are discussed in some detail: n-ZnO/p-NiO, n-ZnO/p-ZCO and n-ZnO/p-CuI.

n-ZnO/p-NiO forms a type-II heterostructure due to the conduction band lineup. Optimized structures exhibit high rectification and exhibit photovoltaic energy conversion combined with high transparency in the visible range ("transparent solar cell"). Only the UV part of the spectrum is converted with an efficiency of 3-4% [2,3]. The heterojunction can also serve as gate in transparent junction field effect transistors (JFET) [4].

n-ZnO/p-ZCO involves a p-type electrode made from amorphous zinc cobalt oxide which is fairly insulating as epitaxial $ZnCo_2O_4$ thin film. In 2014 the high rectification of such diode has been reported for the first time [5]. In the meantime we have reported JFET inverters [6] and JFET ring oscillators (Fig. 1) [7] based on such gate diodes.

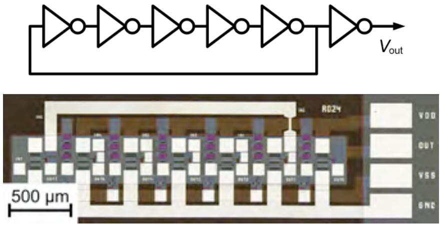

Fig. 1. Schematic and optical image of ZnO JFET-based ring oscillator (ZnO/ZCO gate diodes)

CuI was the first transparent material ever reported (1907) [8] and forms together with n-ZnO highly rectifying diodes [9]. The role of the interface in this type-II heterostructure diode is theoretically modeled and analyzed.

Keywords: diodes; oxide semiconductors; JFET; rectification; interface; transparent electronics

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IMPLEMENTATION OF SILICON NATIVE OXIDE AS A TUNNEL BARRIER FOR SPINTRONICS

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The integration of ferromagnetic and semiconductor materials offer unique possibilities to develop a powerful and reliable method of injecting and detecting spins in the semiconductor material at room temperature. However a strong obstacle for the development of this technology is associated with the large impedance mismatch existent between both types of materials, which limits the spin injection from high conductive ferromagnetic material to high-resistive non-magnetic semiconductor. The use of extremely thin tunnel barriers has been recently proved to be the solution to this problem [1,2]. The use of SiO2 as a barrier is very promising due to its high dielectric constant. However the main problem concerns with the difficulty in stabilizing extremely thin layers of SiO2 on silicon substrates while deposition of the ferromagnetic material.

Within this context, we have successfully grown thin layers of Fe_3O_4 on Si/SiO_2 substrates by PLD, with thicknesses ranging between few nm to 80 nm, in order to determine the applicability of FM-semiconductor integration using SiO_2 native oxide as a tunnel barrier. A complete morphological, compositional, electronic, magnetic and transport characterization has been performed by synchrotron based X-ray reflectivity, high and low energy XPS, Raman spectroscopy, SEM, Magneto-Optic Kerr effect and in-plane transport techniques. Special attention has been paid on the quality of the buried interfaces, thickness of the tunnel barrier and absence of other iron oxide phases or silicate phases. The results showed Fe_3O_4 single phase character without silicate formation, ferromagnetism at room temperature, well-defined metal to insulator transition, high quality interfaces and low tunnel barrier thicknesses.

Keywords: Tunnel barrier; Spintronics.

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A STUDY OF THE ELECTRONIC STRUCTURE OF ENGINEERED SOI MATERIAL

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The extreme demand for the miniaturization and increased performance of electronic devices have led to a search for low dimension, high performance and reliable materials. Silicon has been the preferred choice for decades. Silicon-on-insulator (SOI) consists of a thin Si layer known as the device layer, usually several tens of nanometres in thickness, bonded to a bulk Si wafer with an intermediate insulating oxide layer. When the silicon device layer is very thin, the effective number of atoms contributing to its physical properties are finite and small compared to the bulk. This leads to new electronic, mechanical and thermodynamic phenomena [1]. In order to study the confinement of electrons in SOI, engineered SOI structures were characterized with low-temperature scanning-tunnelling-microscopy (STM) and spectroscopy (STS).

SOIs were cleaned and thinned using plasma techniques [2] and patterned using electron beam lithography. Various scanning tunneling spectroscopic techniques such as field emission [3] and variable height spectroscopy [4] were used to study the varying density of states (DOS) of SOI structures. Significant variation in LDOS were observed for the engineered SOIs. Interestingly, apart from the effects due to low dimension of the structures, parameters such as doping concentration and annealing affects the STM and STS measurements significantly [5]. Further, using electrical measurements and kelvin probe force microscopy (KPFM) we have been able to distinguish and understand these effects. In this work we demonstrate the influence of dopant concentration and quantum confinement in SOI structures.

Keywords: Silicon-on-Insulator (SOI); Scanning tunneling microscopy (STM); Scanning tunneling spectroscopy (STS); Local density of states (LDOS);

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Optical Studies on Flash Lamp Annealed Doped and Undoped β-Ga_2O_3 Thin Films Prepared by Spray Pyrolysis

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With its wide band gap of around 4.9 eV, β-Ga_2O_3 is a promising transparent semiconductor for (opto-) electronic applications. Besides the established techniques for the preparation of β-Ga_2O_3 layers, for instance chemical vapor deposition, electron beam deposition, molecular beam epitaxy, and pulsed laser deposition, low cost techniques such as ultrasonic nebulization and spray pyrolysis are also of great interest. With the latter we prepared β-Ga_2O_3 thin films on silicon substrates.

For the preparation of β-Ga_2O_3 a solution of $Ga(NO_3)_3$ in water or in a water/ethanol mixture was employed. Rare earth elements, like Er^{3+}, Sm^{3+}, and Gd^{3+}, and Al and Mg were used as dopants. The β-Ga_2O_3 thin films were investigated by scanning electronic microscopy (SEM), X-ray diffraction, Raman spectroscopy, as well as imaging and spectroscopic ellipsometry.

Since Gallium oxide, like we prepare it, needs a high annealing temperature to form the β-modification (higher than 800 °C), we use flash lamp for the annealing. There for we use energies from 10 J/cm² to 60 J/cm² and apply some additional heat with a heat plate (room temperature to 600 °C). With this we want to prepare the thin films for the application in (opto-)electronic devices.

In this work we compare by using optical investigations the characteristics of β-Ga_2O_3 thin films, which had been flash annealed and thermal annealed.

FUNCTIONAL THIN FILMS BY DESIGN: EMPLOYING RESONANCE BONDING TO TAILOR THERMOELCTRIC AND PHASE CHANGE MATERIALS

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Phase change and thermoelectric materials utilize remarkable property portfolios, which have made it difficult to design such materials, other than employing trial and error approaches. In this presentation, an alternative is discussed. Phase change materials are characterized by the ability to rapidly switch between the amorphous and crystalline state, which differ significantly in their properties. This material combination makes them very attractive for data storage applications in rewriteable optical data storage, where the pronounced difference of optical properties between the amorphous and crystalline state is used. This unconventional class of materials is also the basis of a storage concept to replace flash memory. This talk will discuss the unique material properties, which characterize phase change materials. In particular, it will be shown that only a rather small group of materials utilizes resonance bonding, a particular flavour of covalent bonding, which can explain many of the characteristic features of phase change materials. This insight is employed to predict systematic property trends and to explore the limits in stoichiometry for such memory applications. It will be demonstrated how this concept can be used to tailor the electrical and thermal conductivity of phase change materials. It even can be utilized to identify thermoelectric materials with large figures of merit. Yet, the discoveries presented here also force us to revisit the concept of resonance bonding and bring back a history of vivid scientific disputes about ‘the nature of the chemical bond’.

IN SITU RAMAN STUDIES OF LASER-INDUCED TRANSFORMATIONS IN Cd-DOPED As_2Se_3 FILMS

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Amorphous As_2Se_3 is a semiconductor material with numerous possible applications related mostly to reversible or irreversible photoinduced effects. Contrary to the extensively investigated amorphous As–Se systems with different As and Se content ratio, studies of doped As_2Se_3, except for the Ge–As–Se systems, are rather rare. Here we report on a study of thin As_2Se_3:Cd films grown by a thermal evaporation technique using atomic force microscopy (AFM), energy-dispersive X-ray spectroscopy (EDX), and micro-Raman spectroscopy.

Thin (1–2 μm) Cd-doped As_2Se_3 films with nominal Cd content of 1 to 10% were grown by thermal evaporation on silicate glass and Si substrates. AFM studies (Agilent AFM 5420) reveal a uniform film surface with a roughness of 0.4–0.8 nm.

EDX measurements (NovaSEM microscope) performed at different electron energies (5–30 keV) show that the content of cadmium gradually decreases from the surface into the film depth. For instance, for As_2Se_3 film with nominal 10 % Cd the cadmium content in the surface layer is 18 %, decreasing down to 2.5 % with probing deeper into the film.

Micro-Raman measurements performed at 295 K using a LabRAM spectrometer and a λ_{exc}=514.7 nm or a λ_{exc}=632.8 nm laser show that at low laser power densities P_{exc} the observed Raman spectra of the Cd-doped films basically reproduce that of the undoped As_2Se_3 films with a dominating broad feature near 225 cm^{-1} that is a clear evidence of their amorphous structure. With increasing P_{exc} a new sharp peak appears at 204–209 cm^{-1} as well as a smaller maximum near 410–420 cm^{-1}. The new peak positions and intensities depend on the Cd content, P_{exc}, and λ_{exc}.

The new peaks in the As_2Se_3:Cd film Raman spectra appear, as a rule, within an acquisition time below 1 min, meaning that the local photostructural changes in the film are quite fast. At relatively low P_{exc} the evolution of the new Raman features with the illumination time can be traced. These changes are irreversible: the new peaks do not disappear after the excitation power is lowered again. This can be explained by the formation of CdSe nanocrystals in the laser spot area: the corresponding LO and 2LO phonon frequencies for CdSe are 210 and 420 cm^{-1}, respectively. The bands are observed in the As_2Se_3:Cd film spectra at slightly lower frequencies because of tensile strain undergone by the nanocrystals due to a photoplastic effect (radial mass transfer from the laser spot) in the films.

Keywords: amorphous thin films; nanocrystals; Raman scattering

THE LATERAL DISTRIBUTION OF OPTICAL PROPERTIES OF CHALCOGENIDE GLASSES MEASURED BY SPECTROSCOPIC IMAGING ELLIPSOMETRY

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Elena Achimova [b), **Alexandra Prisacar** [b),
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Chalcogenide glasses exhibit a variety of properties applicable to optical devices. The vast majority of them are based on photoinduced changes created with band-gap illumination. In particular, the photodarkening, photoinduced surface corrugations and refractive index change are of renewed interest, especially for fabrication of diffractive optical elements or optical fibers.

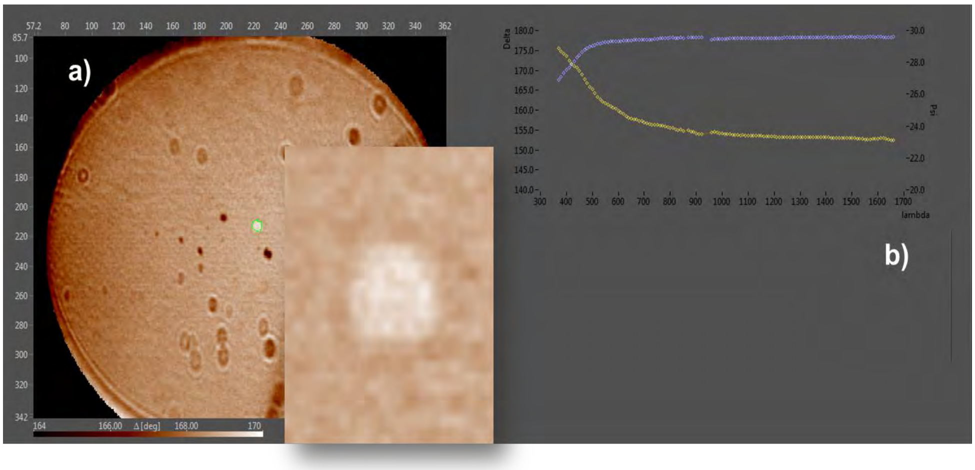

Fig. 1. Delta map (a) and Delta, Psi spectra **(b)** of As_2S_3-Fiber with a core size of 6 μm.

Chalcogenide fibers with core sizes down to 6 μm and holographic gratings with different phase profiles depending on the exposure conditions were characterized by imaging ellipsometry. Ellipsometric enhanced contrast micrographs were used for fast surface inspections. Optical properties of distinctive surface areas were obtained based on regions of interest (ROI) concept. Pattern and profiles of the optical properties were obtained from Delta- and Psi-maps.

To express the dispersion function of chalcogenide glasses mainly a Tauc-Lorentz term was used. In case a roughness layer must be taken into account, a Bruggemann effective medium layer containing chalcogenide glass as host was applied. A main point of view of the work was the characterization of diffraction gratings prepared under parameters that differ from the optimal procedure.

Keywords: Chalcogenide glasses, Imaging Ellipsometry

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REALIZATION OF ORDERED PHASE CHANGE MATERIALS AND THEIR INVESTIGATION VIA ELECTRICAL TRANSPORT, TERAHERTZ AND RAMAN SPECTROSCOPY

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Phase Change Materials (PCMs) are unique compounds employed in non-volatile random access memory thanks to the rapid and reversible transformation between the amorphous and crystalline state that display large differences in electrical and optical properties. In addition to the amorphous-to-crystalline transition, experimental results on polycrystalline alloys evidenced a Metal-Insulator Transition (MIT) attributed to disorder in the crystalline phase.

Here we make use of fundamental advance in the fabrication by molecular beam epitaxy of ordered alloys and heterostructures. We assess the degree of ordering by X-ray diffraction and explicitly correlate it with the MIT by means of electrical transport [1]. We further tune the ordering in a controlled fashion attaining a large range of resistivity. A combination of Terahertz and Raman spectroscopy is employed to investigate vibrational modes and the carrier behavior in amorphous and crystalline ordered epitaxial alloys [2].

Finally, superlattices made of alternating layers are studied by micro-Raman spectroscopy. A structural irreversible transformation into ordered alloys is induced by high power laser light exposure. The absence of this configuration after *in situ* annealing even up to 300°C evidences an electronic excitation induced-transition which brings the system into a different and stable crystalline state [3].

Keywords: PCM; MBE; Raman

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SURFACE PHYSICS BY NODAL LINES IN ALKALINE EARTH METALS

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In the presentation, we study surface physics characteristic in a nodal-line semimetal, which is one of the topological semimetals. We show by ab initio calculations that fcc Ca, Sr, and Yb have topological nodal lines near the Fermi level when the spin-orbit interaction is neglected (Fig.1(a)) [1]. These nodal lines (Fig.1(b)) are purely topological, characterized by the π Berry phase. Because of the topological nature of the nodal lines, the Zak phase, defined as an integral of Berry connection along a reciprocal vector, becomes π within the region (Fig.1 (c)) encircled by the nodal lines. This π Zak phase is related with charge polarization, and it means that there is an excess charge of e/2 or –e/2 within this wavevector region. This charge is screened by bulk carriers, leaving behind a large dipole at the surface and a potential dip at the surface. Eventually, this tends to cause a large Rashba spin-orbit coupling, when atoms with large spin-orbit coupling are added at the surface. It is demonstrated in Bi/Sr(111) surface, as well as in Bi/Ag(111) surface [1].

If time allows, we also show our results on Weyl semimetals (WS) [2], which are topological semimetals with nondegenerate 3D Dirac cones in the bulk. In the presentation we show that if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens [3]. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation [4].

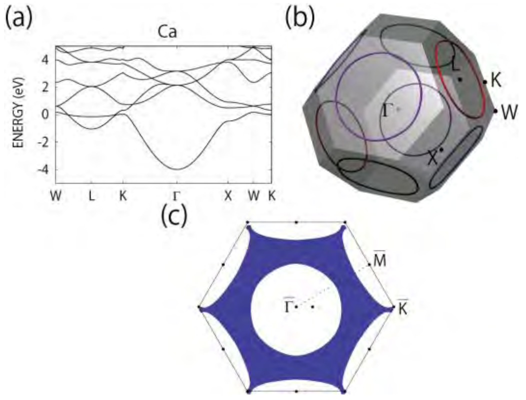

Fig. 1 (a) Band structure of Ca, (b) nodal lines of Ca, and (c) region with π Zak phase on the (111) surface

Keywords: Nodal-line semimetal, Rashba splitting

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UNCONVENTIONAL SPIN TEXTURE IN A QUANTUM SPIN HALL INSULATOR

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CANCELED

Quantum spin Hall (QSH) insulators are materials that let electric current flow across their edge without backscattering while keeping it from passing it through their bulk. This exotic property makes QSH insulators very promising for spintronic devices[1]. Because the predicted QSH insulators have a small bandgap allowing that the bulk states contribute to the electronic transport, the observation and control of topologically protected edge states are one of the major challenges in the current condensed matter physics. We find that, in a nanoribbon of a QSH insulator, both bulk and edge states can be protected by the time-reversal s[illegible]metry. Thus, the backscattering is forbidden at any energy plane for both edge [illegible]lk, allowing the construction of a spintronic device with less energy l[illegible]havior is a consequence of an unconventional spin texture a[illegible]pological properties (Z2=1) and the lack of bulk inversion sy[illegible] and Dresselhaus effects[2]. That is, the bands have th[illegible] We also find a new stable QSH system with this [illegible] This system has a large nontrivial band gap of 0.1[illegible]splitting of 60 meV, which could allow the observatio[illegible]

We would like to thank the financial s[illegible]arch foundation (FAPESP).

Keywords: Topological insulators, Qu[illegible] spin-orbit coupling.

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ANNEALING-INDUCED Bi BILAYER ON Bi_2Te_3 INVESTIGATED VIA QUASI-PARTICLE-INTERFERENCE MAPPING

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CANCELED

Topological insulators (TIs) have much potential for use in practical applications because of their unique electronic properties, wh[illegible] mainly related to two-dimensional (2D) topological surface states (TSS) [illegible] dispersion. Since the TSS of TIs reside within the topmost atomic [illegible] surface, its precise characteristics depends on surface struc[illegible] Hence detailed knowledge of the surface top atomic layers [illegible]

Here we present the morphology chan[illegible] are freshly cleaved in air, upon subsequent sys[illegible] vacuum and the resulting effects on the local and [illegible] of the surface states, which are investigated [illegible] microscopy (STM), scanning tunneling spectro[illegible] spectroscopy (AES) experiments with density fu[illegible]s.

Our findings demonst[illegible] annealing induces the for[illegible] bilayer atop the Bi_2T[illegible] topography of the samp[illegible] Fig. 1. The adlayer [illegible] and the atomic-s[illegible] centers of [illegible] investigated [illegible] surface [illegible]dent quasi[illegible]ping of the su[illegible] and via comparison [illegible] constant-energy conto[illegible] patterns. Our experimental da[illegible]orted by our DFT based calculations of the QPI patterns for the Bi-bilayer fo[illegible]ed Bi_2Te_3.

Fig. 1. Atomically resolved topography after annealing of Bi_2Te_3 in ultra-high vacuum.

Annealing in ultra-high vacuum offers a facile route for tuning of the topological properties and may yield similar results for other topological materials.

Keywords: Topological insulators; Bi_2Te_3; Scanning tunneling microscopy; Density functional theory

Non-equilibrium Surface Dirac Fermion Dynamics of Topological Insulators

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Three-dimensional topological insulators (3D TIs) with surface Dirac fermions in a bulk energy gap induced by a strong spin-orbit coupling have attracted much attention as key materials to revolutionize current electronic devices. A spin helical texture of surface Dirac fermions, where the electron's spin is locked to its momentum, is a manifestation of a 3D TI. To unveil its Dirac fermion dynamics is crucial for the future development of (opto-)spintronic devices incorporating topological insulators. Angle-resolved photoemission spectroscopy implemented by a pump-and-probe method is powerful tool to study both occupied/unoccupied states as well as hot carrier dynamics [1]. Here, the surface Dirac fermion dynamics in the "carrier tuned" topological insulator $(Sb_{1-x}Bi_x)_2Te_3$ have been explored. Sb_2Te_3 (x=0) has a Dirac node completely located above the Fermi energy [Fig.1(*left*)]. The excited electrons in the upper Dirac cone are found to stay longer than those below the Dirac node to form an inverted population. This is attributed to a reduced density of states near the Dirac node [2]. Once the Fermi energy gets into the bulk energy gap by an appropriate Bi doping (x=0.43), the duration of the nonequilibrium surface electronic state exceeds >400 ps. The keys for the prolonged nonequilibration are the bulk insulation and further tuning of the Fermi level to the Dirac point of the topological surface state. These findings expand the pathways to high-mobility opto-spintronic applications.

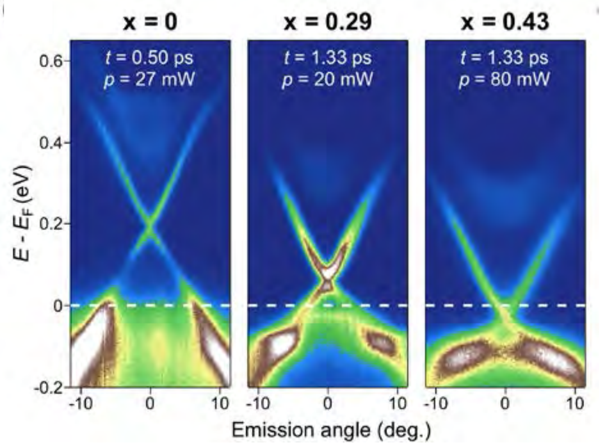

Fig. 1. Band dispersions of $(Sb_{1-x}B_x)_2Te_3$ (x = 0, 0.29, 0.43) acquired at certain pump-and-probe delay times.

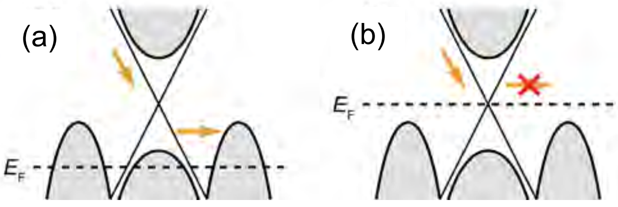

Fig. 1. Schematics of the relaxation processes in bulk metallic (a) and bulk insulating (b) TIs.

The experiments were performed at ISSP, the University of Tokyo (Proposal No. H26/A180, H26/B277, H27/259) in collaboration with K. Sumida, Y. Ishida, S. Zhu, M. Ye, K. A. Kokh, O. E. Tereshchenko, S. Shin. This work was partly supported by the bilateral collaboration program between RFBR (Russia) and JSPS (Japan) and also by KAKENHI No. 26247064.

Keywords: Topological insulators; Nonequilibrium surface Dirac fermion dynamics

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Wednesday:

N112

09:00 *Plenary Talk*: H. Dil

	N112		N113
09:45	*Invited Talk*: S. Facsko	09:45	*Invited Talk*: P. Hofmann
10:45	U. Kreibig	10:45	J.-M. Layet
11:00	D. Erb	11:00	P. H. Thiesen
11:15	R. Zdyb	11:15	Z. Khan
11:30	I. Miccoli	11:30	*Invited Talk*: C. Papp
11:45	H. Holtgrewe		
12:00	~~Z. Li~~		~~K. L. Syres~~

14:00 – 22:00	*Conference Tour & Dinner: Augustusburg Castle*
15:00 – 16:00	*falconer's show*
16:00 – 17:30	*individual visit of a museum*
17:30 – 18:00	*castle chapel with organ presentation*
18:00 – 22:00	*Conference Dinner*

DESIGNING SPIN PROPERTIES IN TOPOLOGICAL, POLAR, AND MULTIFERROIC THIN FILMS

Hugo Dil

Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland
Swiss Light Source, Paul Scherrer Institut, Switzerland

The growth of high quality thin films has since long been known to be an effective method to control or enhance the electronic structure of materials. Here it will be shown that similar considerations can be applied to the spin texture of special classes of materials. For example, in topological insulator thin films the energy position and spatial localization of the spin polarized interface states can be controlled by the adequate choice of substrate and thickness [1].

Furthermore it will be shown that the highly polar surface of the transition metal oxide $SrTiO_3(001)$ hosts a 2D electron gas that exhibits the spin signature of a Rashba-type spin splitting [2]. The properties of this state can be tuned by doping of thin films and transforms into a 2D hole gas for ferroelectric $BaTiO_3$ films.

The previous examples take place at the surface or interface, but the spin degeneracy can also be lifted in the bulk of a thin film if the crystal structure lacks inversion symmetry. In this respect ferroelectric materials bear large promise as in this case the inversion symmetry breaking can be controlled by an external electric field. In the polarized state of ferroelectric GeTe films the electronic structure consists of a plethora of spin-polarized bulk and surface states, whereby the latter can be suppressed by a capping layer [3].

In this work we will take this concept one step further and induce ferromagnetic order in ferroelectric GeTe by Mn-doping. By using a combination of spectroscopic techniques it will be shown that the films are both ferroelectric and ferromagnetic at temperatures below 130K and that the chiral spin texture remains even for Mn concentrations around 20%. Furthermore, our spin-resolved ARPES and soft X-ray ARPES measurements show that the ferromagnetic order induces a Zeeman gap and out-of-plane spin texture around the Dirac point [4]. By switching the magnetization it could be determined that the ferroelectric and ferromagnetic order are directly entangled. This opens up new pathways for the use of non-volatile spintronics applications and electronically switchable magnetic substrates.

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PROPERTIES OF METALLIC THIN FILMS GROWN ON PERIODICALLY CORRUGATED SURFACES

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Nanostructured thin films are of growing relevance for all kind of applications in photovoltaics, plasmonics, or as magnetic materials. Various methods have been used to fabricate nanostructured thin films with well defined morphology exhibiting tunable effective properties. Bottom-up, self-organized methods have been used extensively in the last years because of their fast and easy way of producing large-scale patterns with structures down to 10 nm.

Ion beam sputtering has proven to be a promising way to produce self-organized patterns on various surfaces [1]. Depending on the ion beam incidence angle, hexagonally ordered dot patterns as well as ripple patterns oriented perpendicular or parallel to the ion beam direction are formed during the continuous sputtering. Periodically corrugated surfaces can also be obtained via crystal surface reconstruction during annealing. The resulting surfaces provide templates for the growth of nanopatterned thin films. Depending on the surface and interface free energies these films can grow in a conformal way reproducing the surface topography or as nanoparticles on the substrate surface. Furthermore, depending on deposition angle, substrate temperature, beam flux, and deposition time, the nanoparticles can align parallel to the ripples, eventually coalescing and forming nanowires, thus tuning the physical properties of these structures via their geometrical dimensions.

Metal thin films grown in this way exhibit distinct optical properties due to localized surface plasmon resonance. Due to their alignment along the ripple structures the nanoparticles exhibit strongly anisotropic plasmonic resonances [2]. Furthermore, the magnetic properties of ferromagnetic thin films grown on rippled or faceted substrates are drastically changed by the presence of the periodic structures at the interface and on the surface [3].

Keywords: metallic thin films; magnetic properties; optical properties; surface plasmon resonance

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NANO-SURFACES : SURFACES OF NANOPARTICLES

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Surface Science is usually focused on planar, atomically flat surfaces, which are model systems far from common material specimens. A model system of other kind for surface exploration is the surface of (preferredly spherical nanoparticles (*Nanos*), which is more realistic in the variety of more or less imperfect surface structures, depending on special material choices and particle preparation methods.

They cover a broad field from planar facettes with edges, spikes and corners to disordered or non-crystalline boundaries without any Cartesian symmetry, etc
Such surfaces may be transferred into interfaces (or more precisely: three-dimensional “interlayers”) by foreign embedding media, which may be chosen from inert gases to passive or reactive liquids or to metallic, non-metallic or organic solids,

Their thickness may extend from sub-monoatomic layers to bulk-like surroundings. Those layers exhibit advantages compared to planar systems, since they may cover the interface completely with high uniformity and without any disturbing substrates.

Nanotechnology now-a-days allow the investigation of single such nanos..

Important advantages of this latter research route are extraordinary application sensitivities of many kinds of experiments., mainly due to the huge surface to inner volume ratio of nanos by which surface properties are scaled up. .

However, draw-backs are still to-day problems with sample preparation and characterization, and not all published experiments overcome them convincingly.

Among the most sensitive experiments are plasmonic surface investigations, which, in addition, give insight into the unique nano-size effects observed in the transition region between solid state nanos and molecular ones.
(General properties of surfaces can, however, only be extracted as long as an individual surface / interface can be clearly defined.)

Recent investigations have shown that in plasmonic excitations all electrons both of the inner particle volume and of the whole surface are involved stemming mainly from the conduction energy band but –to lesser extent- also from deeper lying bands and can be separated from each other with help of extensions of the fundamental work of Mie.

Since Mie’s basic paper, concerning spherical surface plasmon polaritons (SPP’s), it was usual to disregard separate surface material properties and to apply instead dielectric functions averaged over the whole particle. To-day we know that material properties of surface regions of nanos may differ essentially from those of the inner volume. Hence, to bring Mie’s description of the SPP’s into quantitative correspondence with experimental results, we require correction - and extension – effect-models concerning special nano-structure - and nano-surface – effects,. which have to be taken into account in the evaluation of the experimental data. .
Most efficient are various extension - effects to describe the observed strong surface induced relaxation and decoherence effects. One important example, the *Chemical Interface Damping* of the SPP’s , will be treated in this contribution to some detail.

It is the purpose of the present paper to compile several such nano-surface corrections which are useful to obtain more precise informations about nano-surfaces and ,moreover, about realistic surfaces in general.

General Reference:

Uwe Kreibig, Michael Vollmer : *Optical Properties of Metal Clusters /* Springer, Berlin 1995

HIERARCHICAL SELF-ASSEMBLY: THREE STEPS TO HIGHLY ORDERED ARRAYS OF UNIFORM METAL NANOSTRUCTURES

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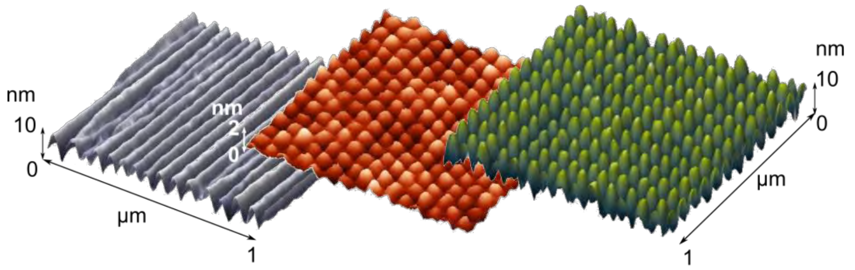
Nanopatterning via self-assembly has gained considerable interest as an alternative to lithography-based techniques for nanostructure fabrication. We propose a procedure for producing highly ordered arrays of uniform metallic nanostructures based exclusively on three subsequent self-assembly processes [1]: crystal surface reconstruction, copolymer microphase separation, and metal diffusion on chemically heterogeneous surfaces. The versatile approach allows for preparing nanostructures with scalable sizes and in a variety of shapes and materials. With this high-throughput technique, nanopatterns covering areas of several square centimeters can be fabricated easily.

We present results of in-situ structural and magnetic investigations of Fe nanodot arrays during formation by grazing incidence small angle X-ray scattering [2] and nuclear resonant scattering of synchrotron radiation [3], examining the dependence of the nanodot shape on deposition conditions and observing the evolution of magnetic moment dynamics during nanodot growth [4]. Possible applications of self-assembled nanopatterns could range from high-density magnetic data storage to catalysis or sensing based on surface plasmon resonance.



faceted α-Al_2O_3 substrate **copolymer template** **self-assembled metal nanostructure pattern**

Figure 1: AFM topography micrographs of the three self-assembling systems combined in the presented procedure. In hierarchical self-assembly, the morphological structures formed in one system guide the structure formation in the following one.

Keywords: self-assembly; diblock copolymers; metal nanostructures

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SPIN-SPLIT ONE-DIMENSIONAL SURFACE STATES ON VICINAL Si SURFACES

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Nanostructures that are supposed to be used in spintronics applications have to fulfill several conditions. Among most important is spin splitting of electronic bands at the Fermi level that is large enough at room temperature to prevent mixing of electrons with the opposite spins. In the present contribution we report on the existence of one-dimensional spin-split metallic states on vicinal silicon surfaces that reveal the largest splitting reported to now at room temperature.

A perfectly regular distribution of steps on a vicinal surface is prerequisite for a good quality of (quasi) one-dimensional nanostructures. The Si(553) surface has been used for this purpose as known to form an array of ordered steps even without any adsorbates [1]. However, in this case the electronic structure does not reveal dispersive and metallic bands, beside the surface state bands similar to those observed on Si(111)-(7x7). Quite different scenario occurs for the surface with the adsorbed Au or Pb atoms. They form either double atomic chains [2] (Si(553)-Au) or nanoribbons [3] (Si(553)-Pb) on each terrace of the vicinal surface.

The presence of the Au or Pb chain-like structures introduces parabolic-like one-dimensional surface states crossing the Fermi level. Due to the strong spin-orbit coupling the bands reveal considerable spin splitting of about 0.2 eV and 0.05 Å^{-1} in case of Si(553)-Au [4] and much larger - 0.6 eV and 0.2 Å^{-1} in case of Si(553)-Pb [5] at the Fermi level. The reason for the difference is a significant anisotropic electron charge distribution around Pb nuclei in the latter case which is caused by the unusual arrangement of the Pb atoms on terraces of vicinal surface [5,6]. It introduces a strong in-plane potential gradient what increases spin splitting of the surface states and the appearance of the out-of-plane component of the polarization vector. The weak interaction between Pb and Si atoms makes the spin-split states well-decoupled from the substrate what should assure pure spin currents in future spintronic devices.

Keywords: Spintronics; vicinal Si; Rashba effect

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QUASI-1D ATOMIC-CHAINS ON VICINAL SURFACES: THE ROLE OF DEFECTS AND CONSTRICTIONS TOWARDS ELECTRONIC TRANSPORT

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Metallic atomic chains on vicinal semiconductor surfaces are prototype quasi-1D ensembles for fundamental research, such as metal to insulator phase transition or Tomonaga-Luttinger liquid behavior [1]. Despite the intense studies over the last decades on several systems, e.g. Si(111)-4x1-In, Si(557)-Au and Si(553)-Au, the effect of native defects or induced by adsorption (e.g. O_2 and H_2) on the conductance of the wires, the interwire coupling or the transition temperature, are still under debate.

Here, we present a systematic study on the transport properties of In- and Au-chains on various Si(hhk) surfaces via a multi-tip STM/SEM system. The conductivities parallel and perpendicular to the wires is quantified by the rotational four-point-probe square method [2]. Additionally, an extremely higher sensitivity towards atomic imperfections and both conductivity components was reached by a spatial constriction of the electron path [2] (Fig. 1a). In detail, the Si(111)-4x1-In system was re-analyzed with greater attention. In contrast to previous studies, we showed in agreement with DFT calculations, that the interwire coupling can be gradually tuned by O_2 adsorption [3] (Fig. 1b). Moreover, the transport properties of various Au-phases on Si(hhk) surfaces were studied. While the 0.48 ML Au on Si(553) turned out to be extremely robust and almost unaffected (up to 20 Langmuir), the 0.2 ML phase on Si(557) reacts strongly as seen by the exponential decrease and the adsorbates induce even a crossover of its conductivity components. The adsorption behavior turns out to be strongly triggered by the presence of a Si-adatom chain, which is a characteristic building block for some Au/Si(hhk) chain systems [4].

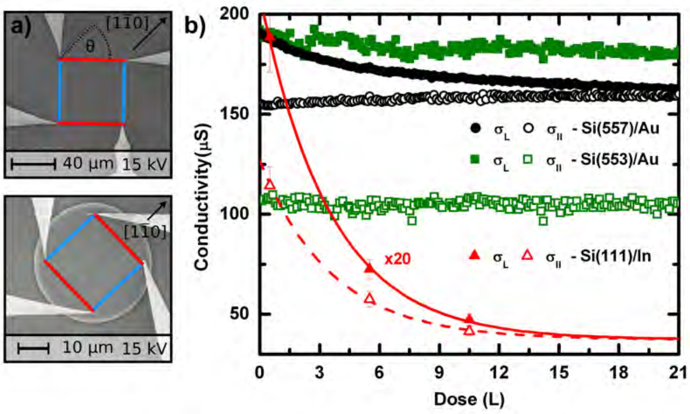

Figure 1: a) STM tips placed in square configuration on an unconfined In/Si(111) surface (above) and confined circular In/Si(111)-mesa structure (below). b) $\sigma_{||}$ and $\sigma_\perp$ versus O_2 dose for the Si(111)-4x1-In system, 0.48ML Au phase on Si(553) and 0.2ML Au phase on Si (557).

Keywords: Atomic-chains, metal-insulator transitions, interwire coupling, defects, lateral constrictions

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DENSITY FUNCTIONAL THEORY INVESTIGATION OF RARE EARTH SILICIDE NANOWIRES

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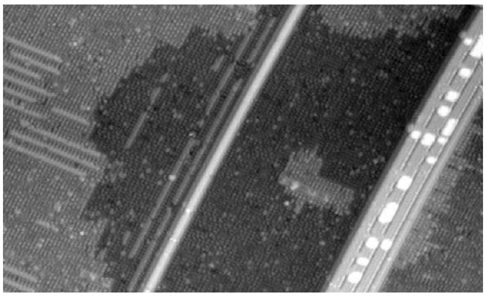

Fig. 1: STM image "showing two broad nanowires at the center and the right of the image as well as some remaining thin nanowires on the left" [1]

Quasi one-dimensional electron systems are of both fundamental interest because of their unusual physical properties as well as potentially interesting for devices on the nanometer scale. In this respect, rare earth (RE) silicide nanowires on silicon (001)-surfaces are of special interest, because the RE silicides exhibit useful physical properties such as low Schottky-barriers, thermal stability and low electrical resistivity one the one hand, and because the silicon (001)-surface is well known and very common in today's technology on the other.

One special feature of the RE silicide nanowires is their preparation, as they grow self-organized controlled by macroscopic parameters such as temperature, deposition amount, and atomic number of the RE. Under variation of these parameters, different systems of RE silicide nanowires have been studied experimentally [1].

Unfortunately, the exact knowledge of their atomic structure, which is crucial for understanding their physical properties, is still incomplete. As a first step towards understanding the nanowires structural and their electronic properties, we have investigated different wire models from first-principles within density functional theory (DFT). Thereby erbium is chosen as prototypical trivalent rare earth ion and its 4f-electrons are treated as frozen state in the atomic core.

The wire models base all on the hexagonal RE silicide structure suggested from the experiment [1]. They have been categorized corresponding to three degrees of freedom, namely width, height and depth of burial. After comparing the formation energy of different models within ab-initio thermodynamics, electronic band structures and densities of states are calculated for the stable wires. Structural and electronic properties are discussed and compared with available STM[1], STS[2] and ARPES[1] measurements.

Keywords: nanowires, rare earth, silicide, DFT

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SIZE-DEPENDENT PENETRATION OF GOLD NANOCLUSTERS THROUGH A NACL MEMBRANE

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Membranes and their size-selective filtering properties are universal in nature and their behavior is exploited to design artificial membranes suited for, e.g., molecule or nanoparticle filtering and separation. Exploring and understanding penetration mechanisms of nanoparticles in thin-film syste[illegible] may provide new opportunities for size selective deposition or embedding of th[illegible]rticles.

Here, we demonstrate an unexpected phenomenon that nonporous atomically thin alkali halide films on a metal support can be exploited as a size-selective inorganic membrane for metal nanoparticles. In particular, relying on scanning tunneling microscopy techniques and density functional theory simulations, we find that NaC[illegible] can filter out larger Au clusters, whil[illegible] clusters are allowed to permeate [illegible] the NaCl onto the Au(111) su[illegible] can be tuned via the thickness of the NaCl film. W[illegible]ism of the filtering effect is the attractive energy/fo[illegible]1) substrate, which forces the clusters to pass thro[illegible]n manner [1].

This mechani[illegible] permeation through any kind of barrier that separa[illegible]ind of attractive force. In particular, the membrane [illegible]u(111) system shows analogy to that of a living bi[illegible]e lipid membrane acts as a barrier for ions and [illegible]ractive force is governed by the osmotic pressure [illegible]vironment. The here observed size-filtering mechan[illegible] understanding nanoparticle-film (membrane) interaction[illegible] nanoparticle filters.

CANCELED

Keywords: Met[illegible]ing, penetration and transmission mechanisms, size-dependent membrane, thin no[illegible] halide film.

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ELECTRONIC STRUCTURE AND ELECTRON DYNAMICS IN NOVEL TWO-DIMENSIONAL MATERIALS

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Changing the dimensionality of a material results in significant modifications of its electronic properties. This is even the case if the parent material already has a layered structure with little interaction between the layers, as in the case of graphene and single-layer transition metal dichalcogenides.

Here we explore the properties of novel two-dimensional materials such as single layers of MoS_2, WS_2 and TaS_2 by scanning tunnelling microscopy angle-resolved photoemission spectroscopy (ARPES). The layers are grown epitaxially on Au(111), Ag(111) and graphene. For the semiconducting materials (MoS_2, WS_2), strong band gap renormalizations are observed due to the interaction with the substrate. For the metallic layers (TaS_2), we can study the effect of low dimensionality on electronic instabilities such as charge density waves and superconductivity.

While the static electronic properties of novel two-dimensional materials can be studied by standard ARPES, investigations of the ultrafast carrier dynamics require both time- and angular resolution and thus time-resolved (TR)-ARPES. There is, moreover, the technical requirement of high photon energies since the interesting part of the aforementioned materials' electronic structure (i.e. the (gapped) Dirac cone) is placed at the two-dimensional Brillouin zone boundary. Recently, it has become possible to probe states at such high *k* by TR-ARPES, thanks to the arrival of ultrafast high harmonic laser sources.

Keywords: Two-dimensional materials, electronic structure, ARPES, STM

FROM MONOLAYER TO MULTILAYER SILICENE

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Silicene has attracted a huge interest since publication of the archetype 3 × 3 reconstructed monolayer phase on a silver (111) substrate in 2012 [1]. It is a synthetic emergent two-dimensional Si-based material that might rival graphene for logic applications in electronics [2] : indeed, the first monolayer silicene device, a Field Effect Transistor with ambipolar characteristics, has been fabricated in 2015 [3].

Ordered hydrogenation of 3 × 3 silicene has been achieved recently in Beijing [4], next in our Lab in Marseille, with further High Resolution Electron Energy Loss spectroscopy results [5].

Multilayer silicene has been also synthesized ; it possesses an intrinsic $\sqrt{3} \times \sqrt{3}$ surface reconstruction, hosts Dirac fermions, and is self-protected in ambient air by its native oxide [6,7]. However, despite such evidences, its mere existence has been severely questioned.

Here, we will show thanks to novel *in situ* Photoelectron Spectroscopy data as well as *ex situ* Surface X-Ray Diffraction and Raman spectroscopy results that multilayer silicene is effectively grown in a rather low temperature regime (~200°C), while, instead, diamond-type silicon terminated by the well-known Si(111)$\sqrt{3} \times \sqrt{3}$-Ag superstructure is formed at higher temperatures.

Keywords: Silicene; 2D Phases; Structural and Electronic Characterizations

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Current Trends in Microscopic Characterization of 2D Materials with Spectroscopic Imaging Ellipsometry (SIE)

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Current developments in the field of 2D-Materials are focused on several areas. These areas include: microscopic devices based on stacking different 2D-materials into hybrid-structures, discovering new material configurations by exfoliating unconventional layered materials, optimizing CVD processes by minimizing crystallite boarders or using ideal shaped microcrystals as the starting point of a growth process and many more. These developments have in common that they require microscopic non-destructive characterization technologies.

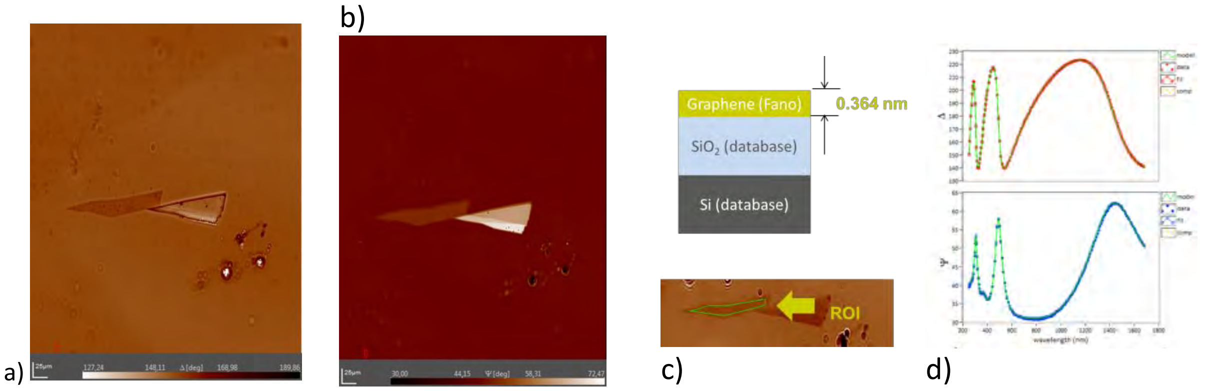

Fig. 1 Spectroscopic imaging ellipsometric measurement of a Graphene flake: Delta (a) and Psi (b) map – examples of a graphene flake, selected Region of Interest and Optical model (c) and wavelength spectra of Delta and Psi, (d) extracted for the ROI from Delta and Psi maps recorded for wavelengths in between 250 and 1700 nm (measured **data displayed as** points and model, line).

Conventional ellipsometry is well established in the field of thin film metrology due to the exceptionally high resolution in the z-axis, enabling very accurate thickness measurements for nano- and microfilms. However, conventional ellipsometry does not have a sufficient lateral resolution for a number of the described developments nor a direct microscopic visualization with highest contrast. The approach of spectroscopic imaging ellipsometry (SIE) differs from conventional ellipsometry in that the measurements are based on a series of micrographs taken at dedicated orientations of the optical components. The primary measurements are microscopic maps of the ellipsometric angles Delta and Psi (Fig. 1 a, b) or micro maps of dedicated elements of the Müller Matrix. Areas can be condensed by binning, averaging of selected pixels data (Region of interest, ROI, Fig. 1c) of equivalent areas and by using histogram data of inhomogeneous regions.

Keywords: Imaging Ellipsometry, Graphene, 2D Materials,

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CHARGE-TRANSFER BETWEEN PLASMONIC NANOPARTICLES AND SINGLE LAYER MoS_2

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Recently, intensive efforts have been made to control the electronic properties of MoS_2 monolayers by doping, including chemical doping[1], gate-bias tuning[2], and physical adsorption[3]. Plasmon-induced hot electrons generated by photo-excitation of Au nanoparticles can also lead to n-type doping of TMDC monolayers[4]. In this contribution, we report on the localized surface plasmons excitation in Au nanoparticles beneath single layer MoS_2. The subsequent changes in vibrational and optical properties of the MoS_2 monolayer were investigated via Raman spectroscopy and photoluminescence in order to evidence the effects of charge-transfer. We report for the first time the visualization as well as the intensity enhancement of the trion peak for this 2D/plasmonic system. Our findings can be effectively driven towards realizing the size and structure of the individual components of opto-electronic devices such as plasmonic field effect transistors.

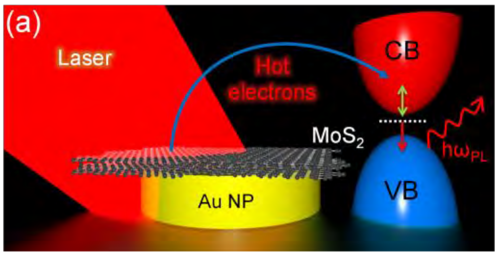

Fig. 1(a): Schematics of the interaction between the Au nanoparticle and MoS_2.

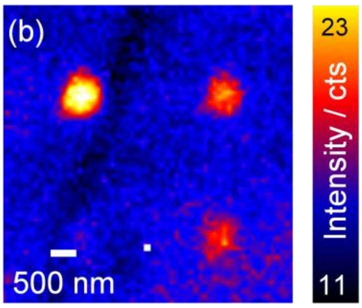

Fig. 1(b): PL intensity map of the 665 nm to 675 nm band showing higher enhancement in the MoS_2 single layer around the Au nanoparticles.

Keywords: MoS_2, plasmonics, hot electrons, two-dimensional, transition metal dichalcogenides, photoluminescence spectroscopy

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MODEL CATALYSIS WITH LIQUID ORGANIC HYDROGEN CARRIERS

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LOHCs are potential candidates for chemical hydrogen storage in future applications: The materials are high boiling organic molecules that can be reversibly hydrogenated and dehydrogenated in catalytic processes. [1] LOHCs consist of a pair of a hydrogen-lean and a hydrogen rich-molecule. The hydrogen-rich molecule is catalytically dehydrogenated at the time and place energy hydrogen/energy is needed, while the hydrogen-lean molecule is hydrogenated in times when excess energy is available.

In this contribution, two examples of the surface chemistry on dehydrogenation catalysts will be discussed, that is, the perhydro-N-ethyl-carbazole (H_{12}-NEC) [2] and dicyclohexylmethane (DCHM) [3]. DCHM and H_{12}-NEC were adsorbed by physical vapor deposition, and subsequently their reaction was monitored during heating. Although the molecules are quite complex, the individual reaction steps were identified by X-ray photoelectron spectroscopy. We will compare the behaviour of the two LOHCs in detail, concerning their dehydrogenation properties. At low temperatures, we find for both the adsorption of a monolayer, followed by formation of multilayers. Upon heating, the multilayers desorb and subsequently distinct dehydrogenation reactions occur, which will be discussed. At elevated temperatures, decomposition reactions are found; these also will be evaluated in detail, since they are detrimental to the storage cycle of the LOHCs.

We acknowledge the Cluster of Excellence “Engineering of Advanced Materials” and the Helmholtz-Zentrum Berlin for the allocation of synchrotron beamtime.

Keywords: Liquid Organic hydrogen carriers, model catalysis, photoelectron spectroscopy.

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NEAR-AMBIENT PRESSURE X-RAY PHOTOELECTRON SPECTROSCOPY OF IONIC LIQUID MULTILAYERS EXPOSED TO WATER; A FUNDAMENTAL STUDY OF GAS ABSORPTION IN IONIC LIQUIDS

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Ionic liquids are composed solely of ions which are held together by a strong Coulomb potential. The large asymmetric ions hinder crystallization causing many to be liquid at room temperature. Ionic liquids have ultra-low vapour pressures and as a result have been studied in ultra-high vacuum conditions using techniques such as X-ray photoelectron spectroscopy (XPS) [1,2]. Ionic liquids [illegible] currently being investigated for applications such as CO_2 capture and stor[illegible]lysis, lubricants, corrosion protection and as an electrolyte in batteries and [illegible] devices [3].

The ordering and structure of ionic liquids is [illegible] constituent ions. For imidazolium-based ionic liquids it has bee[illegible]ange to form a layer of alkyl chains facing towards the [illegible]rlayer containing the anion and the imidazolium ring [illegible]ring at the surface that is believed to govern the ga[illegible] ionic liquids. It is difficult to study the interaction betw[illegible]ecules using conventional XPS under ultra-high [illegible] gas must be pumped away in order to carry o[illegible] pressure X-ray photoelectron spectroscopy (NA[illegible]ing to emerge which allow XPS measurements und[illegible]

In this work, the [illegible]-butyl-3-methylimidazolium tetrafluoroborate, [BMIM[illegible] NAPXPS, as a fundamental study of gas absorp[illegible] multilayers deposited on rutile TiO_2 (110) were [illegible] 283K (corresponding to a relative humidity of 70% [illegible] the University of Manchester. Results indicate tha[illegible] liquid multilayers, causing a disruption and reord[illegible]. As water is pumped out of the near-ambient [illegible] are initially trapped in the ionic liquid layers. When [illegible] ionic liquid layers the ions reverts back to their original st[illegible]

Keywords: Water[illegible]ar-ambient pressure XPS; Gas absorption

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Thursday:

	N112		
09:00	*Plenary Talk*: E. Malic		
	N112		N113
09:45	*Invited Talk*: M. Smerieri	09:45	*Opening – D. R. T. Zahn*
		09:55	S. Klyatskaya
10:45	A. Matkovic	10:45	T. Rüffer
11:00	C. Tegenkamp	11:10	T. Hahn
11:15	*Invited Talk*: W. Auwärter	11:35	V. Kataev
11:45			
13:30	L. Kühl Teles	13:30	C. Hess
14:00	D. A. Evans	13:55	M. Hietschold
14:15	T. Seyller	14:20	S. Tatay
14:30	S. Shah	14:45	P. F. Siles
14:45	C. Noguez		
15:30	C. Wagner	15:30	M. Knupfer
15:45	*Invited Talk*: A. V. Krasheninnikov	15:55	G. Salvan
		16:20	H. Prima-Garcia
16:15	A. C. Ferrari	16:45	F. Zhu
17:00	Poster session		

EXCITONIC FINGERPRINT OF ATOMICALLY THIN 2D MATERIALS

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As truly two-dimensional materials with a weak dielectric screening, monolayer transition metal dichalcogenides (TMDs) show a remarkably strong Coulomb interaction giving rise to the formation of tightly bound excitons. In addition to the optically accessible bright excitonic states, there is also a variety of optically forbidden states including excitons exhibiting a non-zero angular momentum or a non-zero center-of-mass momentum.

Here, we present the excitonic fingerprint in optical absorption and differential transmission spectra based on a microscopic approach that combines the Wannier equation with TMD Bloch equations. We show the appearance of a pronounced Rydberg-like series of excitonic transitions with binding energies in the range of 0.5 eV [1]. We investigate the microscopic origin of their homogeneous linewidth including radiative and phonon-assisted non-radiative relaxation channels [2, 3]. We predict a significant disorder-induced coupling of bright and dark excitonic states offering a strategy to circumvent optical selection rules and make dark states visible in optical spectra [4]. Finally, we study exciton valley dynamics including Coulomb-driven intervalley coupling mechanisms between the high symmetry K and K’ points [5].

Keywords: 2D materials; dark and bright excitons

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FROM ORGANOMETALLIC STRUCTURES TO GRAPHENE NANORIBBONS: DI0042ROMO-PYRENE ON Ag(110)

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In this talk I will discuss our recent results on the formation of low dimensional graphene nanostructures on Ag(110) [1]. By a combination of scanning tunneling microscopy, spectroscopic techniques and density functional theory calculations, we demonstrate the formation of extended, chiral patterns of parallel graphene nanoribbons (GNR) by surface assisted Ullmann coupling and de-hydrogenation [2] of 1,6-dibromo-pyrene. The so-formed polymers are monodispersed in width and show alternated zig-zag and armchair sites at the edges. It’s well known that graphene is a material of exceptional properties, but its intrinsic zero-energy gap reduces the impact for applications in nanoelectronics. On the contrary, GNRs narrower than 10 nm are semiconductors, due to the electron confinement in one dimension and to edge effects [3]. The ability to grow highly ordered nano-ribbons is therefore of relevance for possible applications in nanodevices. Besides that, our result demonstrates the peculiarity of pyrene derivatives for the formation of GNRs on coinage metals, in particular on Ag(110). These results open the possibility of engineering nanostructures of particular shape and dimension (and hence with tailored electronic properties) by choosing suitable molecular precursors. This is further demonstrated by preliminary results on Br-Corannulene self-assembly on the same substrate.

Keywords: Graphene nanoribbons; surface assisted polymerization; dibromo-pyrene Ullman coupling; STM; photoemission spectroscopy; DFT

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EPITAXY OF HIGHLY ORDERED CONJUGATED ORGANIC SEMICONDUCTOR CRYSTALLITE NETWORKS ON GRAPHENE BASED DEVICES

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We focus on the hot wall epitaxial growth of sub-monolayer films of a rod-like conjugated organic semiconductor (OSC), para-hexaphenyl (C36H26, 6P) [1-3], on the surface of graphene based devices. For this purpose, mechanically exfoliated flakes supported by SiO_2/Si substrates are used and contacted in a back-gated two-point probe field effect device configuration.

Charge transfer and doping of graphene channel by OSCs are investigated in situ. Atomic force microscopy (AFM) is used to characterize OSC crystallite morphology (Fig.1a), and Kelvin probe force microcopy (KPFM) is used to investigate changes in the work functions of graphene and 6P crystallites with applied external electric fields (Fig.1b). Furthermore, we show how residues from the lithography and annealing steps affect morphology of the grown OSC thin films.

Van der Waals nature of the interface between OSCs and graphene allows for the growth of crystallites that are several tens of micrometers large, thus minimizing the number of OSC grain boundaries within the device channel, and allowing investigations of the intrinsic properties of the OSCs.

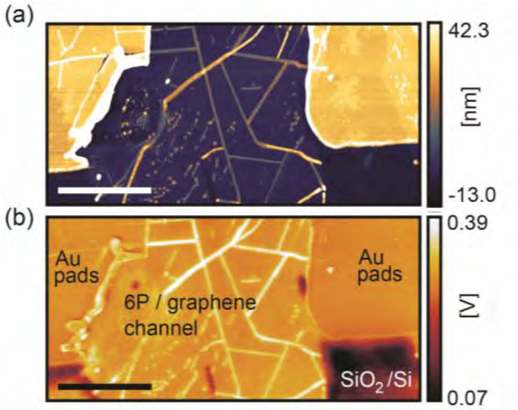

Fig.1. (a) and (b) respectively show AFM and KPFM images of the same 6P/graphene channel area, with grounded back-gate electrode (scale bars 5 μm).

Keywords: hybrid organic/inorganic van der Waals interfaces, charge transfer OSC/graphene, KPFM of OSC crystallites.

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FUNCTIONALIZATION OF EPITAXIALLY GROWN GRAPHENE NANOSTRUCTURES

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Functionalization of graphene is an essential task for any future carbon based electronics. In this respect graphene ribbons grown on pre-structured SiC(0001) surfaces are interesting as they exhibit promising transport properties. Graphene ribbons grown on pre-structured SiC(0001) surfaces exhibit promising transport properties, e.g. high temperature annealing of appropriately designed SiC-Mesa structures results in growth of sidewall nanoribbons revealing robust ballistic transport channels with mean free path lengths up to 16µm at 300K [1]. The existence of edge states on zig-zag oriented ribbons is confirmed by Raman, STM and STS measurements [2,3]. Moreover, by means of STM lithography, we have recently fabricated nano-constrictions within these wires revealing Fabry-Perot like resonance features [4].

Npn-structures with Klein tunneling barriers were realized by functionalizing the buffer layer on top of the SiC-mesas via Ge-intercalation. Depending on the local Ge coverage the chemical potential is either shifted above or below the Dirac point correlating nicely with the morphology as deduced from scanning tunneling microscopy and spectroscopy. The length of a single pn-junction is around 5 nm as revealed by spatially resolved STS measurements and therefore, significantly lower than those induced by field effects. In case of bipolar structures (npn and pnp) the resistance strongly depends on the inner barrier length D. For short barriers (D < 200 nm) the second junction appears almost transparent, a clear signature of Klein tunneling [5].

Keywords: graphene nanoribbons, ballistic transport, Klein tunneling, 4-tip STM SEM

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TETRAPYRROLE MOLECULES ON, AT, AND BELOW EPITAXIAL SP^2-SHEETS

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Atomically thin sp^2-hybridized sheets of hexagonal boron nitride (*h*-BN) can be grown on various single-crystal metal surfaces via chemical vapour deposition, complementing the library of two-dimensional materials including graphene and opening perspectives for van der Waals hetero-structures. *h*-BN monolayers are widely used as templates with the potential to electronically decouple and spatially order atoms, functional molecules and nanostructures.

Here, I will focus on the interaction of tetrapyrrole molecules with sp^2-sheets (*h*-BN, graphene) on Ag and Cu(111) supports. Tetrapyrroles as porphyrins possess an impressive variety of functional properties - including axial ligation, light harvesting and catalytic transformations - that have been exploited in natural and artificial systems. From a surface science perspective, tetrapyrroles are thus ideally suited as building blocks for surface-anchored functional nanostructures [1]. We apply low-temperature scanning tunnelling microscopy (STM), spectroscopy (STS) and non-contact atomic force microscopy (nc-AFM) in an ultra-high-vacuum setting to comprehensively characterize the tetrapyrrole/sp^2 systems with sub-molecular resolution. Specifically, I will address the spatial organization, energy-level alignment, on-surface metallation and coordination reaction of porphyrins on an electronically super-structured h-BN/Cu(111) template [2,3]. Furthermore, an intercalation protocol will be discussed, yielding porphine assemblies buried below a *h*-BN sheet. Given the insulating character of *h*-BN, the covered tetrapyrroles can be addressed by STM. Additionally, we present a dehydrogenative coupling reaction employed to fuse porphines to graphene edges, where distinct bonding motifs are identified by nc-AFM. These approaches provide access to new tetrapyrrole-based systems, metallo-supramolecular arrays and hybrid architectures with prospects for novel, tunable functionalities, e.g., in sensing, heterogeneous catalysis or molecular electronics.

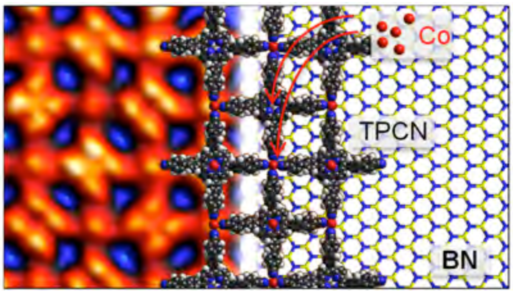

Fig. 1. STM image of a metal-organic coordination network on *h*-BN/Cu(111) formed from functionalized porphyrins (TPCN) combined with Co (left) and schematic model (right).

Keywords: Boron Nitride; Graphene; Porphyrin; Self-assembly, Scanning probe microscopy

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DEPOSITION, ALLOYING AND STACKING OF 2D HONEYCOMB MATERIALS: A VIEW FROM FIRST PRINCIPLES*

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Graphene provided the impact and excitement to explore isolated two-dimensional (2D) crystals, such as hexagonal boron nitride (*h*-BN), transition-metal dichalcogenides (TMDCs), phosphorene, and many others, providing a rich variety in composition, electronic structure and properties. Their unique optical, electronic and mechanical properties make them the next frontier in advanced materials for optical and electronic thin flexible devices applications based solely on 2D layers. Therefore, considerable effort has recently been directed to the synthesis and modification of 2D materials for band gap engineering.

In this talk, I discuss, by means of first-principles electronic structure calculations, the possibilities of synthesizing 2D crystals on a substrate and altering their electronic band structures via different approaches, as alloying and stacking 2D materials vertically, the known van der Waals (vdW) heterostructures. In this context, the following systems are systematically discussed:

(i) The deposition of Sn atoms on top of a Si-terminated 4H-SiC(0001) surface. The influences of the Sn overlayer geometry, the surface passivation by H and F as well as the chemical functionalization of the Sn layer by fluorine and hydrogen, and their topological character are investigated in detail. The explicitly calculation of Z2 invariant shows that the passivation of the substrate is mandatory for obtaining tin based 2D topological insulators.

(ii) The alloying among the group-IV elements [1] and between graphene and *h*-BN are studied considering different local atomic configurations and a statistical method to account for disordered effects, discussing their phase stability through temperature versus composition phase diagrams and predicting the electronic and optical properties.

(iii) The coincidence lattice method derived from surface studies is developed to predict new possibilities for the simulation of vdW heterostructures [2]. This includes finding supercells that require little computational effort to simulate, despite being incommensurable, and assessing combinations with specific rotation angles. This enables theoretical studies to explore deeper possibilities within vdW-bonded systems, effects due to interlayer twist, or Moiré patterns despite limited computational resources. Theoretical structures can be easily created to emulate real-world samples. Results are given and discussed for a variety of the most interesting TMDCs, group IV dichalcogenides, graphene, and group III− V compounds.

**in collaboration with F. Bechstedt, M. Marques, I. Guilhon, D.S. Koda, R. R. Pela and F. Matusalém*

Keywords: first-principles calculations; 2D materials; deposition; alloys; phase separation; van der Waals heterostrutures

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Epitaxial growth of 2d materials by catalytic hexagonalization of diamond and boron nitride.

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There is considerable interest in the fabrication and electronic properties of graphene and related 2d materials such as BN for low-dimensional materials engineering. Like graphene, 2d BN can be fabricated by CVD growth and exfoliation[1]; here we show that it can also be produced by metal-catalysed hexagonalization of cubic BN, in a similar way to the graphitization of diamond.

Advantages of metal-catalyzed graphitization of diamond include the lower temperature in comparison with metal-free graphitization and CVD growth (~ 500°C) and the use of the substrate as a source of material in addition to its use as a lattice-matched substrate. Using photoelectron-based methods[2], we have shown that epitaxy is maintained throughout the process as illustrated schematically in Fig. 1 for graphene growth on the (111) face of diamond.

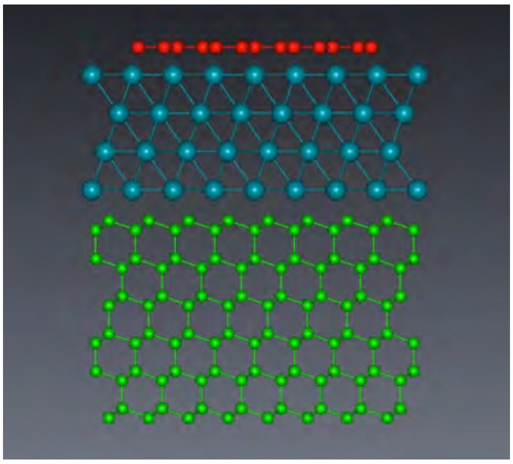

Fig. 1. 2-D growth of graphene (top layer) on a diamond substrate with an interlayer metal catalyst

The graphene grows from below rather than above as in CVD and therefore it is possible to controllably grow single and multilayer films. In a bilayer structure, the inner layer is bound strongly to the metal catalyst, but the second layer exhibits the electron dispersion characteristic of quasi-free graphene with Dirac points at the Fermi level. Using a similar method, we have monitored the hexagonalization of crystalline cubic BN with the same metal catalyst.

Keywords: 2d materials; BN; photoemission

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POLARIZATION DOPING AND WORK FUNCTION OF EPITAXIAL GRAPHENE ON SILICON CARBIDE

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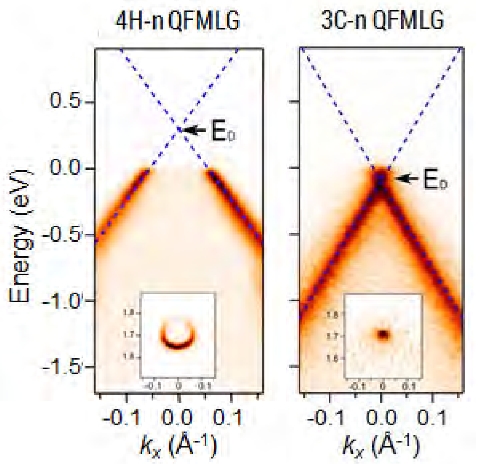

Fig. 1: π-bands of graphene on hydrogen-terminated, n-type 4H-SiC(0001) and 3C-SiC(111) probed by ARPES in the vicinity of the K-point of the hexagonal Brillouin zone. The position of the Dirac point E_D is marked.

Epitaxial graphene grown on SiC surfaces is a promising material for electronic applications such as chemical sensors, THz detectors, quantum resistance standards, etc. The close contact with the substrate has consequences on the properties of graphene. In particular, the epitaxial graphene layers exhibit a characteristic charge carrier density, which can be measured by angle-resolved photoelectron spectroscopy as seen for example in figure 1. The charge carrier density is given by $n = g_S \cdot A_F / A_{BZ}$, where A_F and $A_{BZ} = 7.56$ Å^{-1} are the area of the Fermi surface and the area of the first Brillouin zone in reciprocal space, respectively. $g_S = 2$ is the spin degeneracy. The observed behavior can be explained by interface states, doping of the SiC substrate, and the spontaneous polarization of the SiC substrate [1,2]. Using different polytypes of SiC (cubic 3C and hexagonal 4H and 6H), as well as low-doped (semi-insulating) and highly doped substrates, it is possible to confirm the model.

Besides the substrate induced doping of graphene, its work function is of great importance to understand for example the behavior of contacts and for designing electronic devices. We have determined the work function of single layer and multilayer epitaxial graphene on SiC(0001) using Kelvin probe measurements as well as photo yield measurements. The results indicate that the work function of these systems is directly coupled to the charge carrier density, approaching the value of graphite for increasing layer numbers and charge neutrality.

Keywords: Graphene; silicon carbide; intercalation; doping; work function.

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A UNIVERSAL SUBSTRATE FOR THE STUDY OF TWO-DIMENSIONAL MATERIALS

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The strong research focus that two-dimensional (2D) materials attract since the isolation of single layer graphene in 2004 is giving way to several applications and discovery of unique physical properties not observed in the 2D bulk counterparts [1]. Optical spectroscopy is one powerful tool for the study of these novel materials using SiO_2 on Si that is so far the substrate of choice. That substrate allows the visual inspection of 2D monolayers thanks to the interference of light that provides optical contrast and also enhancement of optical signals [2]. In this work we demonstrate that graphite, as a substrate, offers significant advantages with respect to the usual SiO_2/Si. The possibility to deposit any kind of 2D materials from multilayer, few layers, and monolayers, its chemical purity and stability, the high flatness, and the relatively strong interactions with the 2D materials due to van der Waals forces make graphite an excellent choice as an alternative substrate. We perform a systematic investigation with atomic force microscopy (AFM), photoluminescence and Raman spectroscopy of GaSe, MoS_2, and $ZnIn_2S_4$ deposited on several other substrates (SiO_2, indium tin oxide, and mica) and compare with the superb results obtained using graphite instead (including optical contrast). Moreover, due to the high electrical conductivity of graphite, we also achieved the electrical characterization at the nanoscale using Kelvin probe force microscopy. This work shows an alternative substrate with potential impact in the research of novel 2D materials.

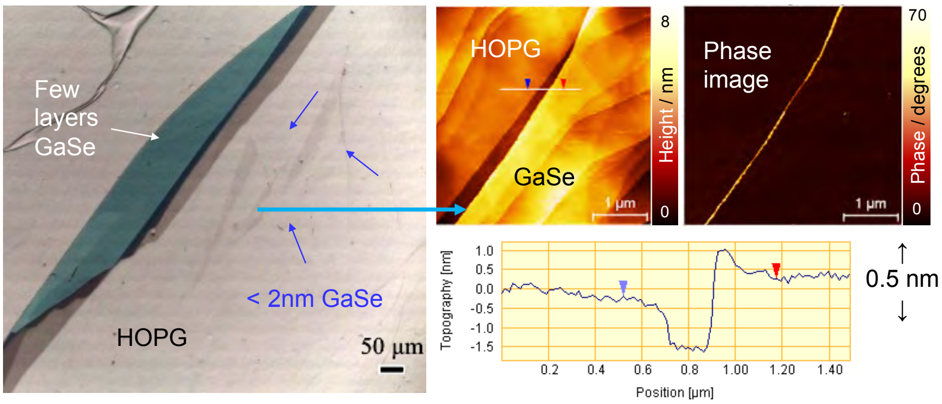

Figure 1: Graphite provides optical contrast in reflection of few layers and monolayers GaSe as dark gray regions. As observed by AFM the GaSe topography follows closely the HOPG. This is an indication of the relatively strong interaction with HOPG that allows deposition of few layers GaSe, that is not so easily accomplished on SiO_2

Keywords: Two-dimensional materials, Raman spectroscopy, photoluminescence, Kelvin probe force microscopy, graphite

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CONTROLLING OPTICAL ACTIVITY IN TWO-ATOM-THICK GRAPHENE

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Recently, the experimental realization of thin films with full control of the structural handedness down to the atomic scale was possible by stacking two graphene layers whose chiral properties are designed by an interlayer rotation angle [1]. The precise handedness can be controlled over several millimeters. This kind of uniform chiral metamaterial with two-atom-thick would provide a powerful tool for exploring and controlling chirality-dependent phenomena, including circular dichroism, templated enantioselective growth in stereochemistry, electronic spin filters in spintronics, among other fields.

In this work, we report theoretical results of the circular dichroism of a chiral stacking of two-dimensional materials are positioned layer-by-layer with precise control of the interlayer rotation. Using a time-perturbed first-principles theory [2], we show that these chiral properties originate from the large in-plane magnetic moment associated with the interlayer optical transition. Furthermore, we show that we can program the chiral properties of atomically thin films layer-by-layer graphene left-handed or right-handed films with structurally controlled CD spectra. The first-principles calculation show that the multipole polarizability, an intrinsic and structure-dependent quantity induced by the chiral nature of the interlayer optical transition, is the origin of the giant optical activity that is comparable to the highest known values for other materials.

Keywords: chiral graphene, 2D-materials, first-principles circular dichroism

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Optical spectra of strained carbon nanotubes: *Ab initio* predictions

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CNTs show unique properties upon strain: Under load, their band gap is opening or closing (depending on the CNTs' chirality) which makes them suitable for electronic and optical strain sensing at the nano scale. Further, they could operate as strain-tunable emitters.

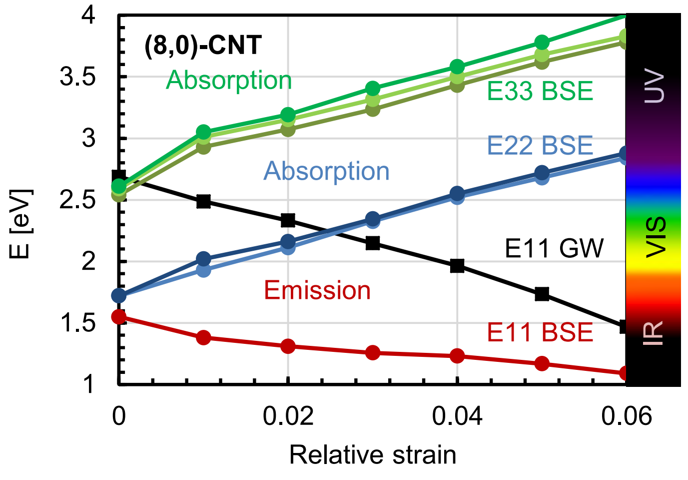

Fig.1: Optical transitions of an (8,0)-CNT on strain.

Our theoretical investigations of strained CNTs show strongly bound excitons that drastically modify the optical spectrum of CNTs with respect to single-particle pictures. The resulting optical transitions strongly shift with respect to strain. However, the shift of the optical transition differs from the shift of the corresponding electronic state. Additionally, the strain-dependent, intrinsic carrier screening alters the exciton binding energy.

Higher optical transitions, depending on their order, shift either in the same or in the opposite direction compared to the first one. This behavior originates from the shift of the electronic bands, which can be qualitatively understood by the tight-binding zone folding scheme. Quantitatively, the exciton binding strength is a function of the band gap and changes on strain. One exemplary result is that the second optical transition of the (8,0)-CNT shifts through the whole visible spectral range if strained up to 5% (see fig. 1).

For our calculations, we use independent-particle (density functional theory, DFT) and single-quasiparticle band structures (G0W0@LDA) to investigate the strain-dependence of the band gap. Further, the Bethe-Salpeter equation is applied for the calculation of the optical spectra in order to describe excitonic effects. In a one-dimensional system, these calculations require the truncations of the Coulomb interaction between periodic images in the supercell approach.

The parameters obtained by these calculations can be used for optical device modeling based on strained CNTs as well as CNT spectroscopy, e.g. infrared spectroscopy, and may allow an extrapolation to other CNTs.

Keywords: Carbon nanotube, ab-initio, optics, strain

DEFECTS IN TWO-DIMENSIONAL INORGANIC MATERIALS

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Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN sheets and transition metal dichalcogenides (TMD) were manufactured. Among them, TMD sheets have received particular attention, as these materials exhibit intriguing electronic and optical properties. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in graphene and inorganic 2D systems obtained in collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials.

Keywords: 2D materials, defects, transmission electron microscopy, first-principles calculations

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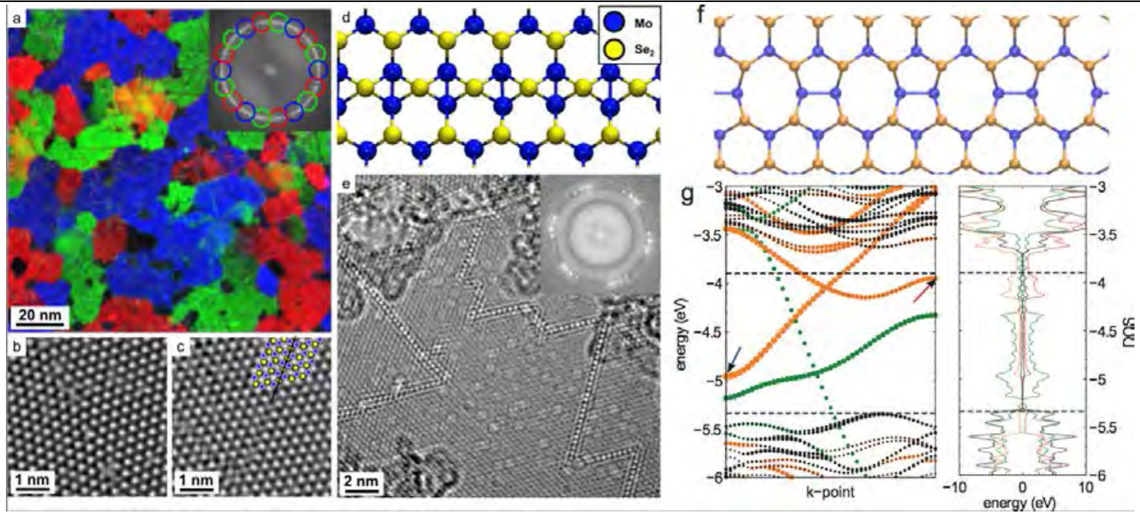

Line defects in inorganic 2D TMDs. (a) The grain structure, with the color coding corresponding to different grain orientations in $MoSe_2$ [from Ref.4]. (b) A close-up view of a tilt grain boundary. c: A close-view of a mirror-twin-boundary within a grain. (d) The theoretical structure, as calculated using DFT. (e) A larger field of view image. Single vacancies are also visible. (f) Atomic structure of another type of mirror twin boundary structure (composed from 5-8 membered rings) observed in WSe_2 [from Ref.1]. (g) Band structure and density of states of a mirror twin boundary in TMD.

Advances in Raman Spectroscopy of Graphene and Layered Materials

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Raman spectroscopy is an integral part of graphene research [1]. It is used to determine the number and orientation of layers, the quality and types of edges, and the effects of perturbations, such as electric and magnetic fields, strain, doping, disorder and functional groups[2,3]. I will review the state of the art, future directions and open questions in Raman spectroscopy of graphene and related materials, focussing on the effect of disorder[3,4], doping[5,6] and deep UV laser excitation[7]. I will then consider the shear [8] and layer breathing modes(LBMs)[9], due to relative motions of the planes, either perpendicular or parallel to their normal. These modes are present in all layered materials[10,11]. Their detection allows one to directly probe the interlayer interactions [10,11]. They can also be used to determine the elastic constants associated with these displacements: the shear and out-of-plane elastic moduli[12]. This paves the way to the use of Raman spectroscopy to uncover the interface coupling of two-dimensional hybrids and heterostructures[10-12].

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MOLECULAR MAGNETISM – A KEY ISSUE FOR QUANTUM TECHNOLOGY

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A major interest in physics, chemistry and materials science is the interface between solid-state physics and functional molecular systems. The bottom-up synthetic approach takes advantage of the intrinsic physical properties of a molecule, of which billions atomically precise copies can be synthesized by chemical methods. Moreover, molecular systems can be organized by surface-confinement and self-assembly protocols using their respective components (organic molecules, metal ions, complexes, etc.) towards complex systems at the organizational level. Beyond this, the molecules often exhibit a wide range of electronic, magnetic, and spintronic properties of fundamental interest and practical importance, thus opening bright avenue towards novel functional nanosystems.

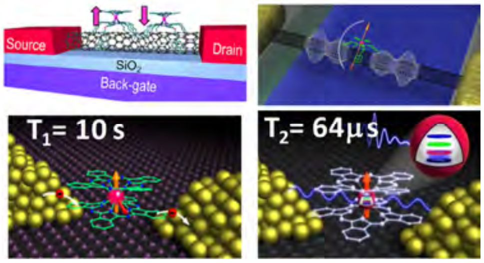

Fig. SMM-based Spintronics Devices

In this talk I will present results from the close collaboration of groups from synthetic chemistry [1, 2] and experimental physics exploring magnetic molecules as building bricks for spintronic devices [3-5]. In this context, the investigation of quantum properties of a single nuclear-spin is a demanding goal. The molecular spin-transistor fabricated allowed for an electrical, non-destructive read-out of the nuclear spin state. Exploiting this property we were able to measure the real-time quantum trajectory of an isolated nuclear spin qubit [6, 7].

Keywords: SMM; Spintronic; Device

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THIN FILMS OF DISCRETE MOLECULES

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Access to the first organic spin valves was reported more than a decade ago and motivated the development of further novel devices as, *for example*, spin-OFETs (Organic Field Effect Transistors).[1] Nowadays, molecules integrated into spintronic devices ranges from diamagnetic molecules to individual single molecule magnets (SMMs).[1] Among them, (metallo)porphyrins or -phthalocyanines are, due to their chemical and thermal stability and the possibility to tune their properties on demand, very promising in terms of application.[1] Hence, selected examples of thin film deposition using porphyrins of the type **H_2**THPP (tetra(p-hydroxyphenyl)porphyrin[2a,b] and **M**TMPP/**H_2**TMPP (tetra-(4-methoxyphenyl)porphyrin, M = Cu[2c], Cu,[2d] Ni[2d]) are reported. Their electronic structure, local transport characteristics and their magneto-optical (MO) properties will be presented. In addition, results obtained for two series of porphyrins of the type **M**TPP(CON(R$_2$)$_4$ (series I/II, cf. Fig. 1) will be presented. Furthermore, novel 2D polymers obtained of **Cu**TPPBr$_8$ on Au(111) (TPP = 5,10,15,20-tetraphenylporphyrin,) will be shown.[3]

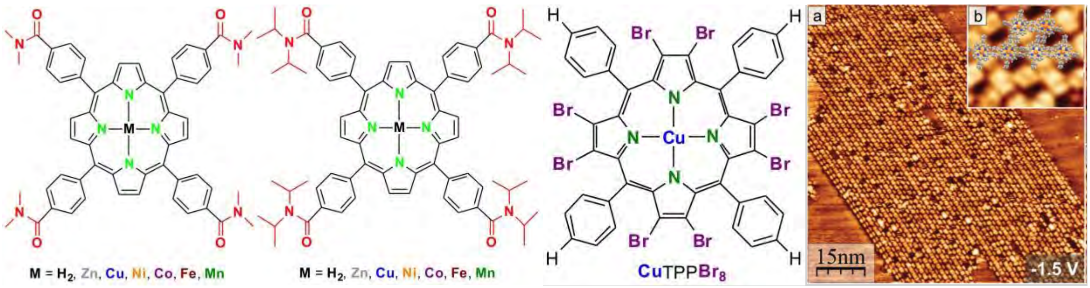

Fig. 1. Chemical structures of **M**TPP(CON(R$_2$)$_4$ porphyrins of series **I** (left) and **II** (middle) and of **Cu**TPPBr$_8$ (right). STM image of an 2D polymer formed of **Cu**TPPBr$_8$ on Au(111) (right).[3]

An alternative approach to fabricate thin films is given in principle by the spin-coating method, a well-established and cost-effective method for diverse applications.[4] However, the formation of smooth thin films of discrete molecules remains challenging.[4] Based on trinuclear bis(oxamato) type complexes a strategy will be presented to overcome this obstacle.[4]

Keywords: (metallo)porphyrins, (metallo)phthalocyanines, trinuclear complexes, molecular and crystal structure, dispersion interactions, spin-coating.

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Transport and charge transfer in metal phthalocyanine hetero structures: theoretical aspects and applications

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Novel charge-transfer compounds formed by combining Metal-Phthalocyanines with different acceptor molecules offer a large variety of physical phenomena and potential applications. Due to the importance of phthalocyanine compounds for fundamental research as well as for future applications it is essential to understand how to modify their electronic properties.

We will present the results of our theoretical first-principle investigations on selected organic charge transfer materials. In particular, we will discuss methodic details about the calculation of charge transfer on pure organic interfaces as well as on organic / metal hetero structures. Further we discuss the implications of charge and spin state changes for typical transport experiments. Such well-controlled tuning of the electrical properties of phthalocyanine junctions stands as key step for future phthalocyanine-based electronic devices. Finally, we will briefly introduce a methodical enhancement to the Density Functional Theory framework that possibly enables the further quantitative description of charge transfer.

This work has been supported by the Deutsche Forschungsgemeinschaft within the Research Unit FOR 1154.

Keywords: Density Functional Theory, Charge transfer, Electronic Structure, Quantum Transport

SUB-THZ HIGH FIELD ESR SPECTROSCOPY ON MAGNETICALLY ACTIVE MOLECULAR COMPOUNDS

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Magnetically active metal-organic molecules that comprise in their cores interacting paramagnetic transition metal ions currently attract a significant interdisciplinary attention due to their unprecedented properties. Some of them provide a realization on a molecular level of a superparamagnetic particle (single molecule magnet) characterized by a big and anisotropic magnetic moment, hysteresis behavior and metastable magnetic states. Such molecular-based materials provide a unique playground to study fundamental aspects of quantum magnetism on the macroscopic level but also there is a need to access them for possible applications in future spin electronic devices. New techniques of tunable sub-Terahertz electron spin resonance spectroscopy in high magnetic fields enable detailed insights into the energy spectrum of the spin states, exchange interactions and anisotropy effects in such kind of systems.

In this talk, ESR studies of transition-metal ion based molecular complexes carried out in the framework of the Saxonian Research Unit “Towards Molecular Spintronics” will be overviewed. It will be shown how the spin-multiplet structure, magnetic anisotropy and exchange interactions can be assessed in the ESR experiment complemented by static magnetic measurements. A relationship between the chemical structure, bonding topology and magnetism of the studied compounds with regard to the rational design of functional materials will be discussed.

SURFACE-GRAFTED PARAMAGNETIC MACROCYCLIC COMPLEXES SEEN BY STM

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The development of molecular nanostructures which contain magnetically bistable transition metal complexes arranged on planar surfaces is an active route towards materials with controllable magnetic or spintronic properties, leading to potential applications on information storage at the molecular level and molecular spintronics. Here we study the molecular anchoring and electronic properties of macrocyclic complexes fixed on gold surfaces [1]. Exchange-coupled macrocyclic complexes $[Ni_2L(Hmba)]^+$ were deposited ex-situ via 4-mer*cap*tobenzoate ligands on the surface of a Au(111) single crystal from solution in dichloromethane. The combined results from STM and XPS show the formation of large monolayers anchored via Au-S *bon*ds with a height of about 1.5 nm. Two apparent granular structures are visible: one related to the dinickel molecular complexes (cationic structures) and a second one related to the counter ions ClO_4^- which stabilize the monolayer. No type of short and long range order is observed. STM tip-interaction with the monolayer reveals higher degradation after eight hours of measurement. Spectroscopy measurements suggest a gap of about 2.5 eV between HOMO and LUMO of the cationic structures and smaller gap in the areas related to the anionic structures.

Paramagnetic Complexes: Self Assembled Monolayers; Scanning Tunneling Microscopy

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TOWARDS UNDERSTANDING AND CONTROL OF ULTRATHIN ORDERED FILMS OF PHTHALOCYANINES AND PORPHYRINES

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Two-dimensionally ordered ultrathin films (mostly monolayers) of various porphyrin and phthalocyanine derivatives on crystalline metallic substrates have been prepared by OMBE. Besides understanding of the self-assembled adsorbate structures observed using STM, also the electronic structure of the films has been studied by STS and PES. Controlled chemical modifications can be performed locally using the STM tip as well as globally using suitable thermal treatment.
Specific examples to be discussed here are:

- Adsorption of metal-free tetra(p-hydroxyphenyl)porphyrin (H_2THPP) on Au(111), Ag (111) and Ag(110) [1];
- STM tip-induced reversible deprotonation of single H_2THPP molecules on Au (111) [2,3];
- Adsorption and heat-induced surface-polymerization of Cu-octobromotetra-phenylporphyrin (CuTTPBr$_8$) on Au(111) [4];
- Self-metalation of metal-free phthalocyanine (H_2Pc) on Ag(110) [5];
- Charge transfer in PtPc-CoPc dimer layers.

An outlook will be given concerning future developments and applications.

Keywords: Ultrathin Organic Films; Adsorbate Structure; Surface Electronic Structure; Porphyrine Derivatives (H_2THPP, CuTTPBr$_8$); Phthalocyanine (H_2Pc); Organic Molecular Beam Epitaxy (OMBE); Scanning Tunneling Microscopy (STM); Scanning Tunneling Spectroscopy (STS); Photoelectron Spectroscopy (PES); Surface Chemical Reaction; Polymerization; Self-Metalation.

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GROWTH OF SELF-ASSEMBLED MONOLAYERS DIRECTLY ON FERROMAGNETIC METAL SURFACES

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Molecular spintronics combines the potential of chemistry with the spin degree of freedom provided by spintronics. In spintronic devices, metal/molecule hybridization can strongly influence interfacial spin properties going from spin polarization enhancement to its sign control [1]. SAMs are composed by a head, a body and an anchoring group that can be independently tuned, thus allowing an easy engineering of the spintronic barrier. In this scenario, while scarcely studied, self-assembled monolayers (SAMs) seem to be the perfect toy barriers to test these tailoring properties in molecular magnetic tunnel junctions (MTJs).

In this communications, we present nanodevices based on alkyl phosphonic acid SAMs used as tunnel barriers and grafted on the half-metallic manganite (La,Sr)MnO_3 (LSMO) [2]. We will present the atypical bias voltage dependence of tunnel magnetoresistance (TMR) highlighting the peculiar role of molecules in the spin dependent tunneling transport. However, as LSMO's surface Curie temperature (Tc) is close to room temperature, spintronics effects in LSMO-based devices are expected only at low temperature. Unlike LSMO, 3d FM metals like Cobalt or Permalloy (Py) have higher Tc but readily oxidize, and additional precautions have to be taken to successfully graft SAMs over them. We will introduce a solution-based grafting protocol for the integration of SAMs and 3d FM metals into spintronic devices. Moreover, we will present the formation of alkanethiol SAMs on Py under inert atmosphere without surface oxidation [3]. Finally, we will show our first results on their integration of SAMs into room-temperature spintronic nanodevices (Fig. 1).

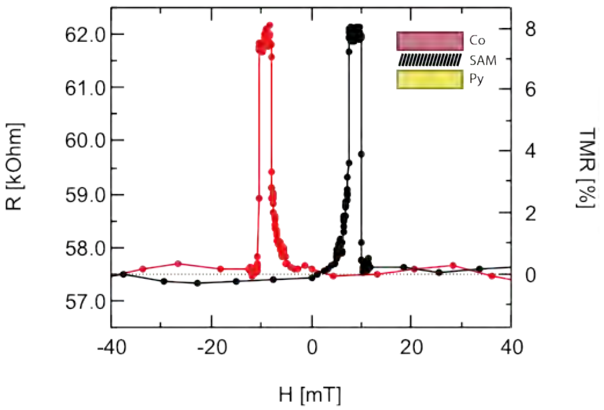

Fig. 1. Magnetic (b) field dependence of conductance measured at 300 K and 40 mV in a Co/SAM//Py junction

Keywords: Spintronics; Self-assembled monolayers

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NANOSCALE TRANSPORT STUDIES OF FUNCTIONAL ORGANIC SYSTEMS

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The charge transport characteristics of organic molecules as well as the ability to control and properly modify these electrical properties represent a key foundation for the field of molecular electronics and the development of novel organic-based electronic devices. In this regard, conductive atomic force microscopy (c-AFM) methods provide unique tools for nanoscale investigations of the plethora of electrical properties provided by organic systems. Here we employ nanoscale I-V spectroscopy as well as spatial electrical current or surface potential mapping approaches to unveil the conducting properties of organic systems which are relevant for device applications.

We correlate the topography and transport properties of metalloporphyrin thin films which present non-homogeneous electrical response due to the formation of nanoscale molecular dendrites and interface defects [1]. We present evidence which allows identifying the proper transport mechanisms of single-molecule magnet systems such as thin films of terbium (III) bis(phthalocyanine) ($TbPc_2$). Here, an electrical spatial mapping of the $TbPc_2$ thin films allows quantifying the charge carrier mobility with nanoscale resolution [2]. We also apply c-AFM methods for the study of the transport properties of important charge-transfer systems such as phthalocyanine-based heterojunctions. The engineering of the organic heterostructure allowed tuning the transport properties as well as identifying transport mechanisms and quantifying the charge carrier mobility of the multilayer systems [3]. A proper understanding of these conditions is fundamental for the search of suitable organic systems and the development of organic-based electronic devices. The approaches presented here represent a starting point towards the development of all-tunable organic-based device technologies.

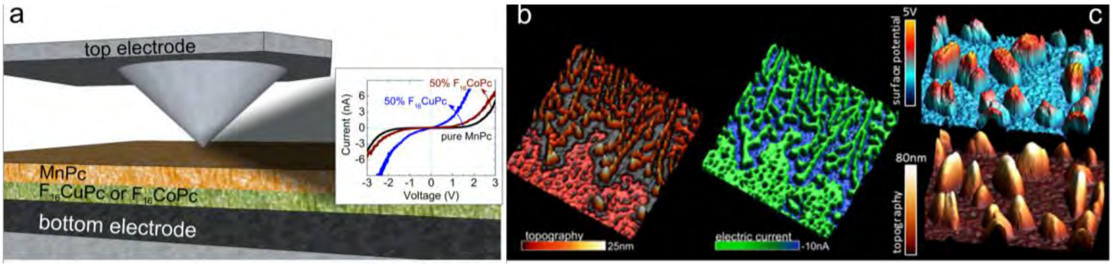

Fig.1. Nanoscale transport studies of organic systems. (a) Tuning of transport characteristics in phthalocyanine thin films *via* incorporation of F_{16}CuPc and F_{16}CoPc. (b) Topography and electrical current correlation on molecular dendrites of metalloporphyrins. (c) Spatial surface potential mapping of VoPc and F_{16}CuPc nanocrystals.

Keywords: conductive AFM; transport properties; organic doping; organic systems

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Charge transfer in Manganese-Phthalocyanine compounds

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Manganese-Phthalocyanine (MnPc) harbors a number of interesting properties, which explains its importance for fundamental as well as more applied research activities. For instance, it is characterized by an unusual S = 3/2 spin state of the Mn^{2+} central ion, MnPc has even been referred to as a typical example of a molecular magnet. Moreover, it shows the smallest ionization potential amongst the transition metal phthalocyanines, and its optical absorption spectrum is far more complex as that of e.g. CuPc.

In this contribution, we will review investigations of charge transfer contributions to the optical absorption data, and the formation of new materials or interfaces based on MnPc, which are characterized by charge transfer reactions. In particular, it is demonstrated that the two energetically lowest absorption features or electronic excitations in bulk MnPc are due to charge transfer excitations, opposite to many other molecular solids where (Frenkel-type) intra-molacular excitations dominate. Further, the formation of MnPc/F_{16}CoPc interfaces is discussed which are characterized by a spin and charge transfer at the interface. Finally, MnPc and the strong electron acceptor F_4TCNQ form a charge transfer (bulk) material in which the MnPc molecules are fully ionized.

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Keywords: Manganese Phthalocyanine, Charge transfer excitations and reactions, Electron Spectroscopy

(MAGNETO-)OPTICAL PROPERTIES OF MAGNETIC MOLECULAR LAYERS

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In this contribution we will provide an overview on investigations of the magneto-optical response of thin films of phthalocyanine molecules on substrates which are relevant for (spin) organic field effect transistors (SiO_2) or vertical spin valves (Co) in order to explore the possibility of implementing phthalocyanines in magneto-electronic devices, the functionality of which includes optical reading.

The optical and magneto-optical properties of phthalocyanine thin films prepared by organic molecular beam depositio [1,2,3] or by spin coating [4] on silicon substrates were investigated by variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect (MOKE) spectroscopy at room temperature. The magneto-optical activity of phthalocyanine molecules in the UV-vis spectral range is determined by the highest occupied and lowest unoccupied molecular orbitals and their hybridization degree with the central metal ion. In addition to the details of the molecular electronic structure, the growth mode and hence the molecular orientation with respect to the substrate can dramatically tune the magneto-optical activity. In the case of phthalocyanine films, the tuning of the molecular orientation can be achieved by controlling the substrate surface properties via the substrate treatment [1] or via exploiting a templating effect introduced by ultra-thin molecular layers or by using metallic ferromagnetic substrates (Co).

Our observations open new perspectives for combining magnetism and optics in devices such as spin-OFETs and organic spin valves. The change in polarization state of a linearly polarized light beam reflected by an active layer of $TbPc_2$ might be used as a diagnosis tool for eventual electronic changes under applied electric/magnetic field in a spintronic device.

Keywords: phthalocyanines; porphyrins; magneto-optical response

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Modulating light emission in a spin-OLED through spin injection at high voltages

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Spin-based electronics is one of the emerging branches in today's nanotechnology and the most active area within nanomagnetism. So far spintronics has been based on conventional materials like inorganic metals and semiconductors. Still, an appealing possibility is that of using molecule-based materials, as components of new spintronic systems [1]. In particular, by taking advantage of a hybrid approach one can integrate molecular materials showing multifunctional properties into spintronic devices. In this talk we illustrate the use of this approach to fabricate multifunctional molecular devices combining light and spin-valve properties (i.e., Spin-OLEDs). So far only one report has been published which is based on the fabrication of an organic light emitting diode (OLED) with ferromagnetic electrodes [2]. Our approach is based on the use of a HyLED (Hybrid Light Emitting Diode) structure in which LSMO and Co are used as ferromagnetic electrode. This device works simultaneously as a spin valve and an electroluminescent device at low temperatures [3]. This new approach leads to a robust organic luminescent device in which light emission can be enhanced and modulated upon application of an external magnetic field (Figure 1)

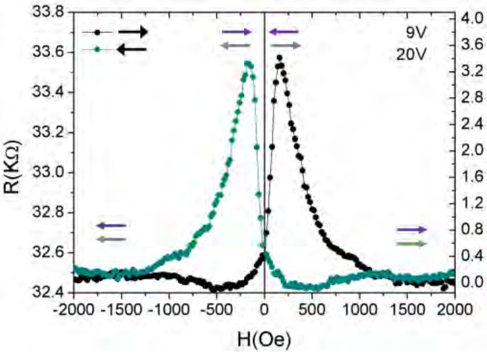

Figure 1. *Magnetoresistance at 9 V and 20K of the PEIE SO. Black arrows depict the field sweep direction. Purple and grey arrows point the FM electrodes magnetization direction.*

Molecular Spintronic, Spin-OLEDs, multifunctional devices

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ORGANIC NANOSTRUCTURE DEVICES BASED ON ROLLED-UP NANOMEMBRANES

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Over the past decades organic nanostructures have attracted huge interest due to their importance in understanding fundamental properties and creating molecular electronic/spintronic nanodevices [1, 2]. Normally, molecular nanodevices rely on electronically connecting molecules through the formation of metallic electrodes. However, the fragile nature of molecules make it difficult to realize nondestructive metal/organic contacts when the metal electrode layers are fabricated by conventional methods of metal deposition, thereof the development of molecular nanodevices has been severely restricted. In this talk we will summarize the contribution from our project team towards the objectives of the TMS research group. A novel robust contact method based on strained and rolled-up nanomembranes will be introduced after shortly reviewing the state-of-art 'soft' contact techniques for molecular devices [3]. The fabrication of self-assembled-monolayer (SAM) diodes and spin-valves structures consisting of non-destructive (ferromagnetic) metal/organic interfaces will be demonstrated. Furthermore, the local investigation via atomic force microscope (AFM) techniques and the application of organic nanocrystal diodes for sensing NO_2 will be discussed [4, 5].

Keywords: Nanomembrane, Rolled-up technology, Organic nanostructure, Organic spin valves

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Friday:

	N112
09:00	*Invited Talk*: H.-P. Steinrück
09:30	*Invited Talk*: B. Kersting
10:30	*Invited Talk*: C. Kumpf
11:00	*Plenary Talk*: R. Wiesendanger
11:45	Closing session
12:15	… *Departure*

SURFACE CHEMISTRY IN COMPLEX ORGANIC LAYERS

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Chemical reactions on surfaces can be followed in detail using X-ray photoelectron spectroscopy (XPS or ESCA), in particular in combination with scanning tunneling microscopy (STM). From the XPS binding energies of the adsorbate and substrate core levels, detailed information on the chemical composition, chemical state (e.g. oxidation state), adsorption sites, but also on the photoemission process itself can be derived. STM provides information on surface order and intramolecular conformation but also on the chemical state. Based on the understanding obtained for simple adsorbate systems, now complex molecular systems can be studied in great detail. One specifically interesting group of materials are metalloporphyrins. These metallotetrapyrrole complexes are versatile functional building blocks in many biological and biochemical processes. Moreover, there are several examples where such molecules were utilized in technical applications, retaining their highly functional nature within an inorganic framework. Examples include gas sensors, solar cells and catalysts. In this presentation the surface chemistry of porphyrins on metal and oxide substrates will be addressed. Specific topics are the interplay between porphyrin-substrate and porphyrin-porphyrin interactions, the role of the substrate, surface diffusion, and the synthesis of metalloporphyrin monolayers by direct metalation of free base porphyrins.[1-7]

Keywords: Porphyrins; Metalation; XPS; STM

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CHEMISORPTION OF EXCHANGE-COUPLED METAL COMPLEXES ON GOLD VIA AMBIDENTATE CARBOXYLATO LIGANDS

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A novel strategy for the fixation of redox-active dinickel(II) complexes with high-spin ground states to gold surfaces was developed. The dinickel(II) complex $[Ni_2L(Cl)]ClO_4$ (where L represents a macrocyclic ligand) was reacted with ambidentate 4-(diphenylphosphino)benzoate (dppba) or 4-mercaptobenzoate (mba) coligands to form the carboxylato-bridged complexes $[Ni_2L(dppba)]^+$ (**2**) and $[Ni_2L(mba)]^+$ (**3**), which can both be isolated as perchlorate or tetraphenylborate salts. The auration of the complexes was probed on a molecular level, by reaction with AuCl or $[AuCl(PPh_3)]$, which leads to the monoaurated $Ni^{II}_2Au^I$ complexes $[Ni^{II}_2L(dppba)Au^ICl]ClO_4$ (**4**) and $[Ni^{II}_2L(mba)Au^IPPh_3]^+$ (**5**), respectively. The bridging thiolate-functions of the N_6S_2 macrocycle are deeply buried and are unaffected/unreactive under these conditions. All complexes were fully characterized by ESI mass spectrometry, IR and UV/Vis spectroscopy, X-ray crystallography, cyclic voltammetry, SQUID magnetometry and HF-ESR spectroscopy. Temperature dependent magnetic susceptibility measurements reveal a ferromagnetic coupling between the two Ni(II) ions in **2**-**5** with J values ranging from 15 - 23 cm^{-1}. HF-ESR measurements yield a negative axial magnetic anisotropy ($D < 0$) which implies a bistable (easy axis) magnetic ground state. The binding of the $[Ni_2L(dppba)]ClO_4$ complex to gold was ascertained by four complementary surface analytical methods: contact angle measurements, atomic force microscopy, X-ray photoelectron spectroscopy and spectroscopic ellipsometry. The results indicate that the complexes are attached to the Au surface via coordinative Au-P (or Au-S) bonds in a monolayer.

Keywords: Macrocyclic Ligands / High-Spin Molecules / Chemisorption / Ambidentate Phosphorus Ligands / Gold / Surface Complex

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GROWTH, INTERACTION PHENOMENA AND PHASE DIAGRAM OF HETEROMOLECULAR ADSORBATES ON METAL SURFACES: THE MODEL SYSTEM PTCDA+CUPC/AG(111)

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Interfaces between organic semiconductors and metals have been investigated intensively in order to improve and develop future electronic devices. In this context the formation of molecular blends (i.e., heteromolecular layers containing at least two different types of molecules, usually charge donors und acceptors) on metal surfaces is of great interest. In this context, we have so far investigated structural and electronic properties of prototypical systems (PTCDA, NTCDA and several metal-Phthalocyanines on noble metal surfaces) using LEEM/PEEM, LEED, STM, NIXSW, ARPES, orbital tomography and STS.

Here we report a novel thermodynamic phase diagram for molecular blends formed by PTCDA+CuPc on Ag(111). In the submonolayer regime, two homo- and three heteromolecular ordered structures occur with different stoichiometry. Large eutectic regions exist in the phase diagram, caused by the opposite intermolecular interaction of the components – repulsive for CuPc, attractive for PTCDA. We find that the repulsive species cause the formation of a 2D lattice gas, the density of which determines the stability of all other phases. Critical values of the gas-phase density are the basis for understanding this constant-volume phase diagram that perfectly describes our experimental observations. We envisage the general validity of this type of phase diagram for binary systems containing gas-like phases.

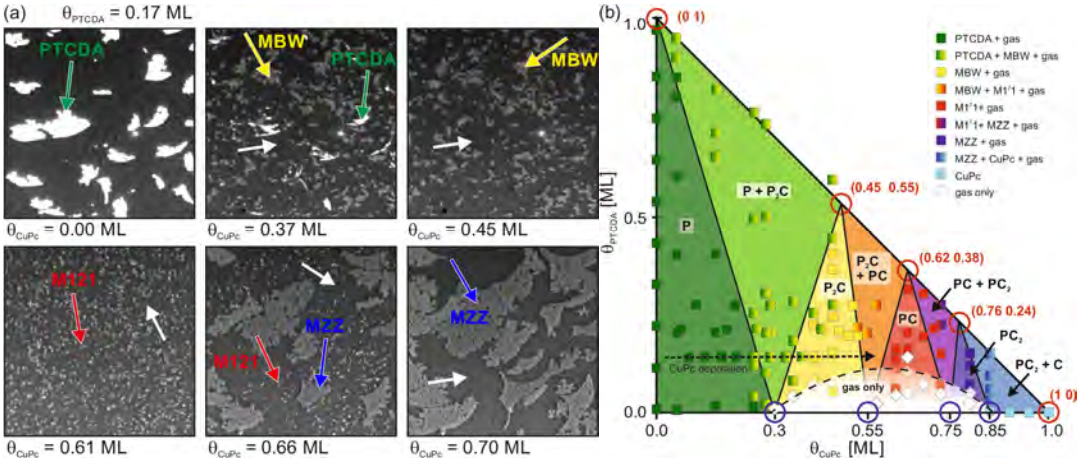

Fig. 1. (a) Bright-field LEEM images recorded during deposition: Initially, the Ag(111) surface is covered by 0.17 ML PTCDA (upper left image). Subsequently, 0.7 ML CuPc were deposited, as shown by the following five LEEM images. The original PTCDA islands (marked by green arrows) are sequentially transformed to MBW (yellow), M121 (red) and MZZ islands (blue), according to the stoichiometry sequence. (b) Phase diagram for PTCDA/CuPc heteromolecular submonolayer structures at 300K: Experiment and thermodynamic model. Colored areas and data points mark the regimes of pure and eutectic phases as obtained from model and experiment, respectively. A dotted arrow indicates the path of the experiment shown in (a). The model is based on more than 20 LEEM experiments with different initial coverages. Abbreviations: P = PTCDA, C = CuPc; Sequence and stoichiometry of the phases: PTCDA (P) – MBW (P2C) – M121 (PC) – MZZ (PC2) – CuPc (C).

Keywords: metal-organic interfaces, molecular blends, phase diagram, LEEM/PEEM

NOVEL INTERFACE-INDUCED ELECTRONIC AND SPIN STATES REVEALED BY SPIN-RESOLVED SCANNING TUNNELING SPECTROSCOPY

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Recently, exotic states of ultrathin films resulting from interfacial interactions have become of great interest in various fields of nanoscience research. As first example, nanoscale magnetic knots, called skyrmions, will be discussed which represent novel types of localized non-collinear spin textures offering great potential for future energy-efficient magnetic memory and logic devices [1]. The twisting in the skyrmions' magnetization profile leads to a gain in energy with respect to a homogeneously magnetized, ferromagnetic state. As a result of this magnetization twisting, skyrmions have non-trivial topological properties. The energetics of skyrmionic states in ultrathin films is explained by the interfacial Dzyaloshinskii-Moriya interaction [2] being relevant in material systems exhibiting large spin-orbit coupling and a lack of inversion symmetry. By using atomic-resolution spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy (SP-STS) [3] we have shown that magnetic skyrmions in ultrathin film systems can be as small as one nanometer in diameter [4] and that their properties can largely be tuned by the choice of the substrate and overlayer materials [5,6]. By locally injecting spin-polarized electrons from an atomically sharp SP-STM tip, we are able to write and delete individual skyrmions one-by-one, making use of spin-transfer torque exerted by the injected high-energy spin-polarized electrons [5]. Alternatively, individual skyrmions can be created and deleted by local electric fields, which can be of great advantage in view of energy-saving skyrmionic device concepts.

As second example, we will focus on interfacial superconductivity in novel types of heterostructures. Here, we present an SP-STS study of ultrathin $FeTe_{1-x}Se_x$ ($x = 0, 0.5$) films grown on prototypical Bi-based bulk topological insulators. We observe fully developed U-shaped superconducting gaps in $FeTe_{0.5}Se_{0.5}$ layers of one unit cell (UC) thickness with a transition temperature (Tc) of ~11 K, close to the one of the corresponding bulk system (Tc ~ 14.5 K). Surprisingly, we also find clear evidence for superconductivity up to Tc ~ 6 K for one UC thick FeTe layers grown on Bi_2Te_3 substrates, in contrast to the non-superconducting FeTe bulk compound which exhibits bicollinear AFM order in a wide temperature range up to 70 K. Even more surprisingly, detailed investigations of the atomic-scale spin-resolved local density of states by SP-STS reveal that superconductivity in one UC of FeTe grown on Bi_2Te_3 appears to spatially coexist with bi-collinear AFM order. This finding opens novel perspectives for theoretical studies of competing orders in Fe-based superconductors as well as for experimental investigations of exotic phases in heterostructures of topological insulators and superconducting layers.

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Poster Contributions

[Poster_01] Milekhin, A. G.
"AU NANO- AND MICROANTENNA ARRAYS FOR SENSOR APPLICATIONS FROM MID-INFRARED TO TERAHERTZ"

[Poster_02] Selyshchev, O.
"THE INFLUENCE OF DOPANT LOCALIZATION ON THELUMINESCENCE PROPERTIES OF CE(III) AND EU(II)-DOPED ZNS AND SRSNANOPARTICLES"

[Poster_03] Kalbacova, J.
"QUANTIFYING DEFECTS IN CARBON BASED NANOMATERIALS"

[Poster_04] Wolff, S.
"INTERCALATION OF EPITAXIAL GRAPHENE ON SIC(0001) BY ANTIMONY"

[Poster_05] Parmar, D.
"CHEMICAL REACTIVITY AND DOPING INVESTIGATION OF GRAPHENE WRINKLES USING RAMAN SPECTROSCOPY"

[Poster_06] Okano, S.
"INVESTIGATION OF DEFECTS IN GRAPHITE BY MICROSCOPIC ELLIPSOMETRY"

[Poster_07] Schütze, A.
"GROWTH AND CHARACTERIZATION OF THIN MOS2 LAYERS ON EPITAXIAL GRAPHENE ON SIC(0001)"

[Poster_08] Dehnert, M.
"SUBSURFACE IMAGING OF FUNCTIONALIZED AND POLYMER GRAFTED GRAPHENE OXIDE"

[Poster_09] Néel, N.
"DEPOPULATION OF SINGLE-PHTALOCYANINE MOLECULAR ORBITALS UPON PYRROLIC-HYDROGEN ABSTRACTION ON GRAPHENE"

[Poster_10] Balle, D.
"INTERACTIONS OF TRANSITION METAL PHTHALOCYANINES AT METAL SURFACES – INFLUENCE OF INTERCALATED GRAPHENE BUFFER LAYERS"

[Poster_11] Anselmo, A. S.
"PHOTODEGRADATION OF PCBM AND C60 FILMS"

[Poster_12] Antonio, C. A.
"COATING CONTAINING MG-DOPED HYDROXYAPATITE PRODUCED BY PLASMA ELECTROLYTIC OXIDATION"

[Poster_13] Evans, D. A.
"MODIFYING DIAMOND SUBSTRATES BY THE CONTROL OF SURFACE OXYGEN COMPOSITION"

[Poster_14] Sharif, R.
"IN-SITU STUDY OF THE FIRST STEP’S OF COPPER OXIDE FORMATION ON CU (110) ELECTRODE SURFACE"

[Poster_15] Henderson, Z.
~~*"ADSORPTION AND DESORPTION BEHAVIOR OF AN IONIC LIQUID ON ZN-TERMINATED AND O-TERMINATED ZINC OXIDE SURFACES: AN ANGLE-RESOLVED PHOTOEMISSION STUDY"*~~

[Poster_16] Rangel, R. C. C.
"CORROSSION RESISTANCE OF CARBON STEEL COATED WITH A SIOX-ORGANOSILICON LAYER"

[Poster_17] Kröger, P.
"SURFACE TRANSPORT ON THIN SEMI-METALLIC FILMS: THE ROLE OF FILM THICKNESS AND MAGNETIC IMPURITIES"

[Poster_18] Bortchagovsky, E.
"OPTICAL PROPERTIES OF SELF-ORGANIZED NANOSTRUCTURED HYBRIDE FILMS DOPED BY RHODAMINE 6G"

[Poster_19] Klump, C.
"SELECTIVE NUCLEATION OF MNSB ISLANDS ON GAAS SUBSTRATES"

[Poster_20] Geurts, J.
"RAMAN SPECTROSCOPY OF THE LATTICE DYNAMICS AND CRYSTAL FIELD SPLITTING IN CEPT5 LAYERS ON PT(111)"

[Poster_21] Arnay, I.
"MAGNETISN OF FE3SI FILMS AND ITS CORRELATION WITH ITS CRYSTALLOGRAPHIC PROPERTIES"

[Poster_22] Evans, D. A.
"STRUCTURE AND BONDING CONTROL IN ULTRATHIN IRON FILMS"

[Poster_23] Sklyadneva, I. Yu.
"SURFACE DYNAMICS OF 0.5-1 ML PB ON CU(111)"

[Poster_25] Reddy, A.
"PHOTOTHERMAL AND VIBRATIONAL MAPPING OF SURFACES AND INTERFACES BEYOND THE DIFFRACTION LIMIT OF LIGHT"

[Poster_26] Banayeem, H.
"THE ROLE OF TIP-SAMPLE INTERACTION IN TIP-ENHANCED RAMAN SPECTROSCOPY IMAGING"

[Poster_27] Seino, K.
"AB INITIO CALCULATIONS AND INFRARED PLASMONIC INVESTIGATION OFMETALLIC PROPERTIES OF THE SI(111)-(5X2)-AU SURFACE"

[Poster_28] Seino, K.
"FIRST-PRINCIPLES CALCULATIONS OF AU-INDUCED WIRE STRUCTURES ON GE(001) SURFACES: NEW ATOMIC MODELS FOR HIGHER AU COVERAGES"

[Poster_29] Teles, L. K.
"COINCIDENCE LATTICES AND INTERLAYER TWIST FOR OPTIMAL VAN DER WAALS HETEROSTRUCTURES"

[Poster_30] Emminger, C.
"MODEL DIFFICULTIES FOR PREDICTING THE POLARIZATION SENSITIVE REFLECTED SECOND HARMONIC GENERATION"

[Poster_31] Dues, C.
"AB-INITIO INVESTIGATION OF RARE-EARTH SILICIDE THIN FILMS ON SI(111)"

[Poster_32] Mukherjee, A.
"TOWARDS EFFICIENT PLASMONIC EXCITATION OF METAL NANO-ANTENNAS AS AN EFFECTIVE TOOL FOR TIP-ENHANCED RAMAN SPECTROSCOPY"

[Poster_33] Solonenko, D.
"HYDROGENATION OF SILICENE PHASES ON AG(111)"

[Poster_34] Zerson, M.
"SURFACE STRUCTURE OF SEMICRYSTALLINE NAPHTHALENE DIIMIDE-BITHIOPHENE COPOLYMER FILMS STUDIED WITH ATOMIC FORCE MICROSCOPY"

[Poster_35] Göhler, F.
"ELECTRONIC AND STRUCTURAL PROPERTIES OF FERECRYSTALLINE COMPOUNDS INVESTIGATED BY PHOTOELECTRON SPECTROSCOPY"

[Poster_36] Rahaman, M.
"STABILITY OF GASE MONOLAYERS"

[Poster_37] Gomonnai, O. O.
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Au NANO- AND MICROANTENNA ARRAYS FOR SENSOR APPLICATIONS FROM MID-INFRARED TO TERAHERTZ

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Energies of localised surface plasmon resonances (LSPR's) in metal nanostructures can be located in the spectral range from ultra-violet to terahertz depending on their size and morphology. It allows them as key element for surface-enhanced infrared absorption (SEIRA) by organic and inorganic materials to be used.

Here we present the results of an investigation of SEIRA by semiconductor nanocrystals (NCs) and organic substances homogeneously deposited on arrays of Au antennas and show the effectiveness of antenna for detection of an ultra-low amount of matter.

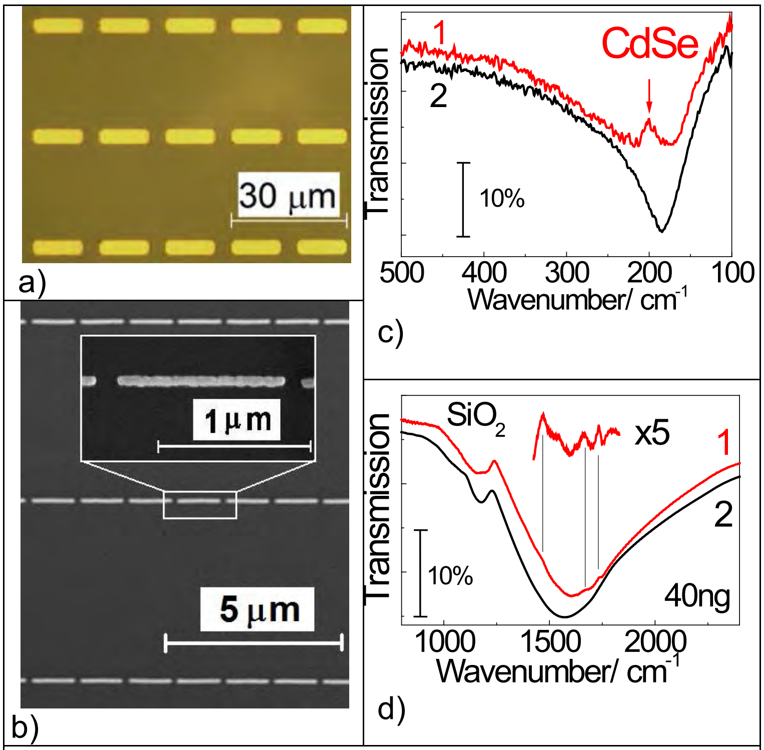

Fig.1 a)- Optical and b)-SEM images of Au nanoantenna arrays. SEIRA spectra of c)- 1 monolayer of CdSe nanocrystals and d)- 40 ng of cortisol. The IR spectra of the virgin arrays (curves 2) are given for comparison.

Nano- and optical lithography was employed to fabricate Au antenna arrays on a Si surface with specific structural parameters, i.e. length and width (Fig.1a,b), providing an energy of the localised surface plasmon resonance (LSPR) close to that of the most intensive vibrational modes in the organic molecules and optical phonons in semiconductor NCs (Fig.1c,d). The structural parameters of Au antennas were determined by scanning electron (SEM) and optical microscopy. The LSPR energy in the arrays of Au antennas as a function of their size was determined by means of IR spectroscopy. The potential of nanoantenna arrays for determining the cortisol concentration in real biological samples is discussed.

This work was supported by Russian Science Foundation (project 14-12-01037).

Keywords: enhancement; IR absorption; phonons

THE INFLUENCE OF DOPANT LOCALIZATION ON THE LUMINESCENCE PROPERTIES OF Ce(III) AND Eu(II)-DOPED ZnS AND SrS NANOPARTICLES.

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Luminescence of semiconductor and dielectric nanoparticles doped with rare earth ions are of interest due to their potential applications as biomedical sensors and as fluorescent components in color screens and white light emitting devices (LEDs) [1,2]. One of the fundamental problems associated with doped nanoparticles is the influence on their properties of the large percentage of surface atoms. In current study we try to answer what way the location of Ce(III) and Eu(II) in a volume or on a surface will influence on their luminescence by doping of zinc and strontium sulfides nanoparticles.

Nanoparticles were obtained by single source precursor method by decomposition of dithiocarbamate complexes of Strontium, Zinc, Europium (III) and Cerium (III) in high boiling point solvents. By successive addition of complexes in reaction mixture there were synthesized two series of nanoparticles: ZnS@Eu^{2+}, SrS@Eu^{2+}, SrS@Ce^{3+} and ZnS@Eu^{2+}@ZnS, SrS@Eu^{2+}@SrS, SrS@Ce^{3+}@SrS where the ions of dopants are localized respectively on the surface and in the volume between the core and the shell layers consisting of the same substances.

For ZnS@Eu^{2+} nanoparticles it was observed a red luminescence at 645 nm, whereas for ZnS@Eu^{2+}@ZnS luminescence was vanished. So one can conclude that luminescence of ZnS activated by Eu^{2+} is caused by surface location of Eu^{2+}.

In a case of SrS activated by Eu^{2+} a red luminescence was observed for both SrS@Eu^{2+}@SrS and SrS@Eu^{2+} nanoparticles with emission maxima at 610 and 580 nm respectively. In excitation spectra of SrS@Eu^{2+}@SrS it was found two bands attributed to own Eu^{2+} 4f–5d electronic transitions and probably to SrS host excitation with subsequent energy transfer on Eu^{2+} ions. For SrS@Eu^{2+} only own 4f–5d Eu^{2+} excitation was detected. This differences may be referred to changes in the local environment of Eu^{2+}.

In luminescence spectra of SrS@Ce^{3+}@SrS NP a green emission with duplet at 480 and 530 nm was observed which attributed to 5d-4f Ce^{3+} electronic transitions. The duplet was originated due to spin-orbit coupling of $4f^2$ configuration of Ce^{3+}. The SrS@Ce^{3+} nanoparticles were showed only weak luminescence in region 450-600 nm which may be caused by the light emission of organic stabilizing agents on the surface of the nanoparticles.

Keywords: luminescence; surface; volume; zinc sulfides; strontium sulfide; cerium; europium.

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QUANTIFYING DEFECTS IN CARBON BASED NANOMATERIALS

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One of the important challenges in integrating single-wall carbon nanotubes (SWCNTs) into new applications is to be able to characterize and quantize defects. For the case of carbon based materials, Raman spectroscopy proved to be an appropriate tool to evaluate the defect concentration or the defect type.
Our aim is to investigate defects in graphite and SWCNTs induced by highly focused gallium ion beam source. The changes in the Raman spectra (D, G, G' bands) are followed with two laser excitation lines (514.7 and 632.8 nm). We show the evolution of Raman spectra with doses from $2\cdot10^{10}$ to 10^{15} ions/cm^2. To compare graphite to other carbon nanomaterials and its behaviour due to the irradiation, we prepared thin films of electronic type sorted – highly enriched semiconducting and metallic - SWCNTs. For all materials a pattern was created in order to statistically evaluate the role of defects.
As such, we have proven that the I_D/I_{G+} intensity ratios derived from Raman spectroscopy is quantitative measure of the defect concentration.

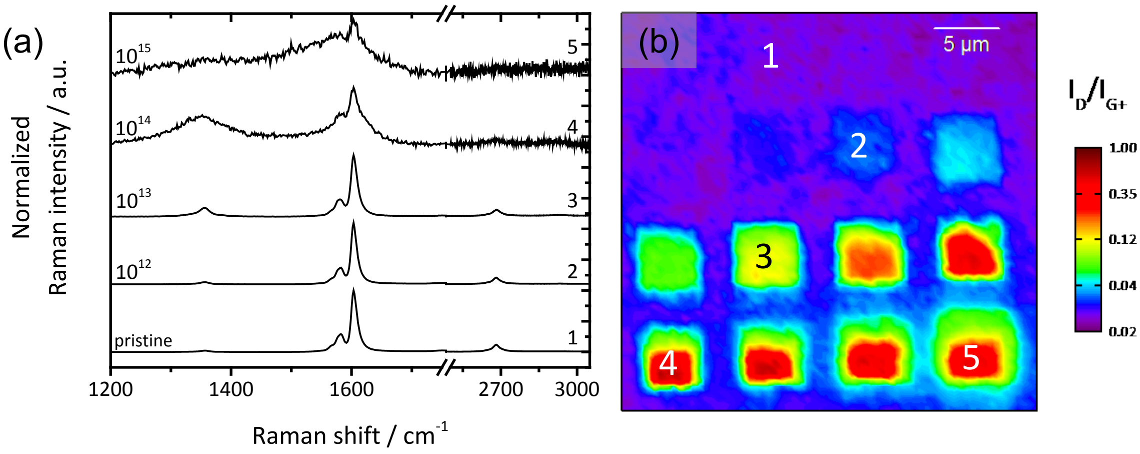

Fig. 1. Selected Raman spectra of carbon nanotubes exposed to increasing ion doses (a). 3D representation of the intensity ratio of D and G$^+$ bands (b). The ion dose is increasing from the upper left to the right and from the top to the bottom.

Keywords: graphite, carbon nanotubes, defects, Raman spectroscopy, focused ion beam

INTERCALATION OF EPITAXIAL GRAPHENE ON SiC(0001) BY ANTIMONY

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Sublimation growth of graphene on SiC(0001) in argon atmosphere presents a well-established method for the preparation of graphene up to wafer scale [1]. This method leads to an interfacial graphene-like layer – the buffer layer (BL) – which is covalently attached to the substrate. Consequently, it lacks the electronic properties typical of graphene. The BL, however, can be detached from the SiC by intercalation, resulting in quasi-freestanding graphene. In addition, the electronic properties of graphene can be tuned by intercalation as well.

We use x-ray photoelectron spectroscopy and angle-resolved photoelectron spectroscopy to investigate intercalation of antimony, which has been predicted by theory [2]. Sb is deposited on the BL by molecular beam epitaxy. Whereas subsequent annealing in ultra-high vacuum results in re-evaporation of Sb without intercalation, Sb remains on the sample upon annealing in argon at atmospheric pressure at comparable temperatures (Fig. 1). Successful intercalation of Sb is evidenced by core-level spectroscopy, demonstrating the conversion of BL to graphene (Fig. 2).

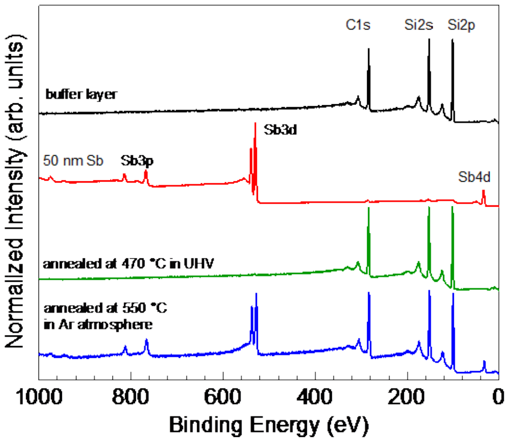

Fig. 1. Survey spectra of pristine BL, BL after deposition of 50 nm Sb, and after annealing in UHV and Ar.

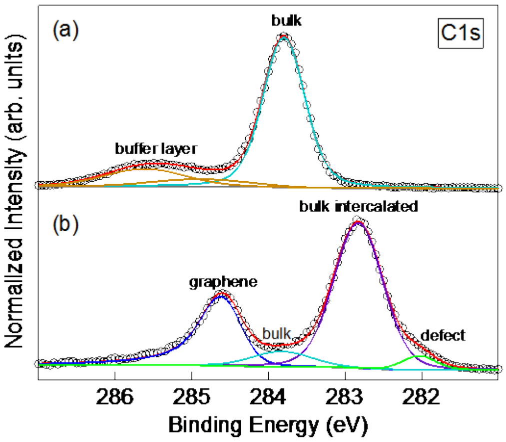

Fig. 2. C1s spectra of BL (a) before and (b) after intercalation of Sb.

Keywords: Graphene; Intercalation; Silicon carbide; Photoelectron spectroscopy

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CHEMICAL REACTIVITY AND DOPING INVESTIGATION OF GRAPHENE WRINKLES USING RAMAN SPECTROSCOPY

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Graphene is attracting much attention owing to its superior electrical, mechanical, thermal, and optical properties. Chemical vapour deposition (CVD) is a well-established method. CVD of graphene on low cost copper foil is the most prominent method for the large-scale growth of graphene. However, a particular issue of CVD graphene on copper is the presence of wrinkles. These wrinkles can contribute to the chemical reactivity and also to changes in the electronic properties of graphene. In our experiments, we have used pristine graphene prepared by CVD method on cooper and then transferred on SiO_2 substrate. Here, we investigated the chemical reactivity of basal plane and wrinkle on graphene functionalized with polystyrene bromide (PSBr). Moreover, we correlate defect concentration and doping of the different regions in graphene. For reactivity investigation, we used Raman spectroscopy and atomic force microscopy to determine the defects and structural morphology. Furthermore, we can also correlate morphology and chemical reactivity to find out how much morphology of wrinkles can affect chemical reactivity of graphene. According to our results, the wrinkles dominates the chemical reactivity of CVD graphene. Therefore, understanding the differences in chemical reactivity of wrinkles in CVD graphene could help engineering novel opto-electronic applications.

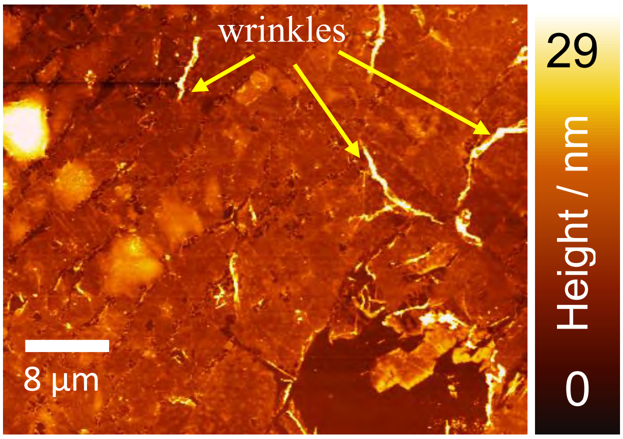

Fig. 1. Atomic force microscopy topography image of graphene functionalized with PSBr.

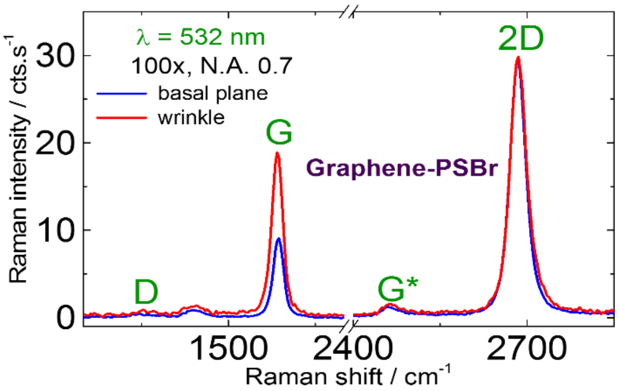

Fig. 2. Raman spectra of functionalized graphene with PSBr comparison basal and wrinkle.

Keywords: graphene, wrinkle, Raman spectroscopy, chemical vapor deposition, polystyrene bromide (PSBr)

Investigation of Defects in Graphite by Microscopic Ellipsometry

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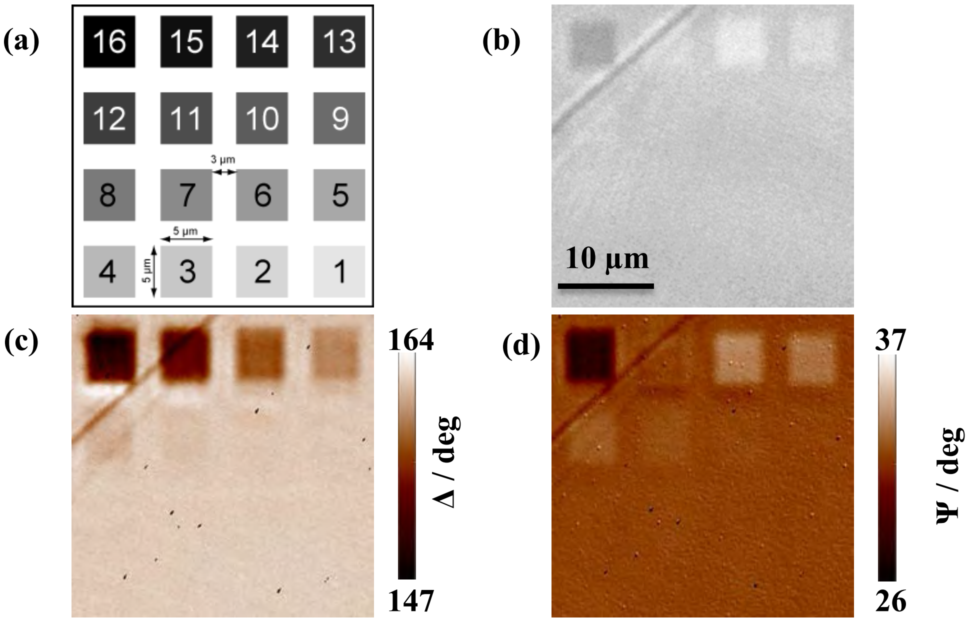
Carbon materials, like graphite, graphene, and carbon nanotubes, are very interesting for many technological applications. Since crystalline affect impact the physical properties, such as the refractive index and optical absorption, in this contribution we present a complementary investigation of defects in graphene by microscopic spectroscopic ellipsometry with an Accurion Nanofilm EP4 setup and micro-Raman spectroscopy and imaging. Defects were produced in square arrays of 5×5 □m^2 on highly ordered pyrolytic graphite by a focused Ga$^+$ ion beam. The defect concentration was varied by controlling the ion fluence from $3{\cdot}10^{10}$ to 10^{15} ions/cm. While Raman spectroscopy imaging provided information on defect concentration and changes in crystallinity and sp^2 hybridization of carbon in graphite, ellipsometry allowed determine the changes in optical properties and its correlation with defects as seen in the Δ and Ψ difference in Figures1(c) and (d), respectively. This work and the complementary approach we used contribute to the understanding of defects in carbon-based nanomaterials and their impact on optical properties.



Keywords: Graphite, Micro Imaging Ellipsometry,

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GROWTH AND CHARACTERIZATION OF THIN MoS_2 LAYERS ON EPITAXIAL GRAPHENE ON SiC(0001)

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The unique property of layered metal dichalcogenides such as MoS_2 to transform from an indirect to a direct semiconductor when reducing the thickness to one monolayer offers new possibilities for electronic devices. For applications, however, the availability of scaleable production methods is a prerequisite.

In the present work, we investigate the chemical vapor deposition (CVD) of thin layers of MoS_2 using sulfur powder and two different molybdenum precursors, MoO_3 [1] and $MoCl_5$ [2]. MoS_2 was deposited on monolayer graphene (MLG) epitaxially grown on SiC(0001). Alternatively, the so-called buffer layer (BL), which is a graphene-like layer strongly bound to SiC(0001) [3], was used as substrate. Both BL and MLG were prepared by sublimation growth in argon at atmospheric pressure as described elsewhere [4].

Samples were characterized using X-ray photoelectron spectroscopy (XPS) for the chemical composition of the samples, atomic force microscopy and low-energy electron diffraction for the structure and crystallinity of the deposited layers. For MoO_3 as precursor, a rather inhomogeneous MoS_2 growth is found which is accompanied by interface oxidation of the SiC due to oxygen intercalation. On the other hand, $MoCl_5$ as precursor results in an improved homogeneity of the deposited films and sulfur intercalation as suggested by XPS data. For the latter, a thickness of the deposited MoS_2 of approximately 1 to 3 monolayers is derived from analysis of core-level intensities.

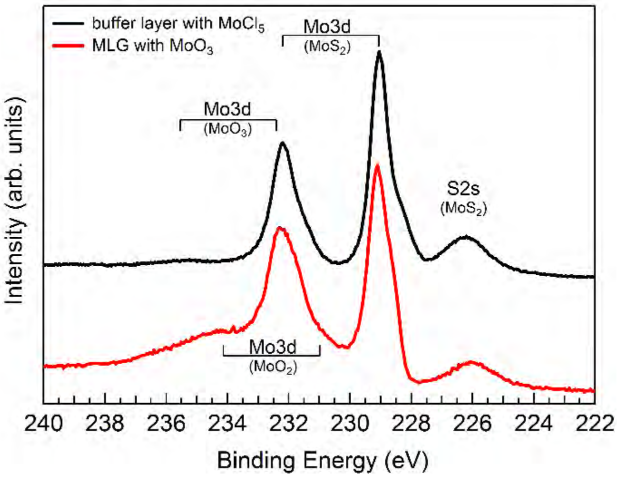

Fig. 1. Mo3d and S2s core-level spectra of CVD-MoS_2 films on buffer layer and monolayer graphene using $MoCl_5$ and MoO_3 precursors, respectively.

Keywords: MoS_2; Graphene; CVD; XPS

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SUBSURFACE IMAGING OF FUNCTIONALIZED AND POLYMER GRAFTED GRAPHENE OXIDE

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We investigate the surface and subsurface morphology of stearylamine modified graphene oxide sheets and polystyrene-grafted functionalized graphene oxide sheets using atomic force microscopy (AFM) operated in multiset point intermittent contact mode.[1] This allows for depth-resolved mapping of the nanomechanical properties of the top surface layer of the functionalized graphene oxide sheets.

On the surface of stearylamine functionalized graphene oxide sheets [2], we can distinguish areas of hydrophilic graphene oxide from hydrophobic areas functionalized with stearylamine. On the latter, larger repulsive forces act on the AFM tip and these areas are more deformable than the not functionalized graphene oxide surface. Measuring the height of several layers of graphene oxide and functionalized graphene oxide, we find that every single sheet of graphene oxide is functionalized with stearylamine on both sides of the sheet. The stearylamine coverage increases the bending stiffness of the stearylamine functionalized graphene oxide sheets which show no wrinkles.

Exposure of polystyrene-grafted functionalized graphene oxide [2] to chloroform vapor during the AFM measurement causes a selective swelling and a softening of the polystyrene envelope. Depth resolved mapping of the tip-sample interaction allows imaging the shape of the folded and wrinkled graphene oxide sheets within the polystyrene envelope; furthermore, it allows measuring the thickness of the swollen polystyrene envelope. This yields the swelling degree, the grafting density, and the chain conformation of the grafted polystyrene layer.

Our work demonstrates a versatile methodology for imaging and characterizing on the nanometer scale functionalized and polymer-grafted graphene oxide and other two-dimensional materials.

Keywords: Graphene oxide; surface modification; grafted polystyrene; swelling; chloroform; 3D-depth profiling; atomic force microscopy

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DEPOPULATION OF SINGLE-PHTALOCYANINE MOLECULAR ORBITALS UPON PYRROLIC-HYDROGEN ABSTRACTION ON GRAPHENE

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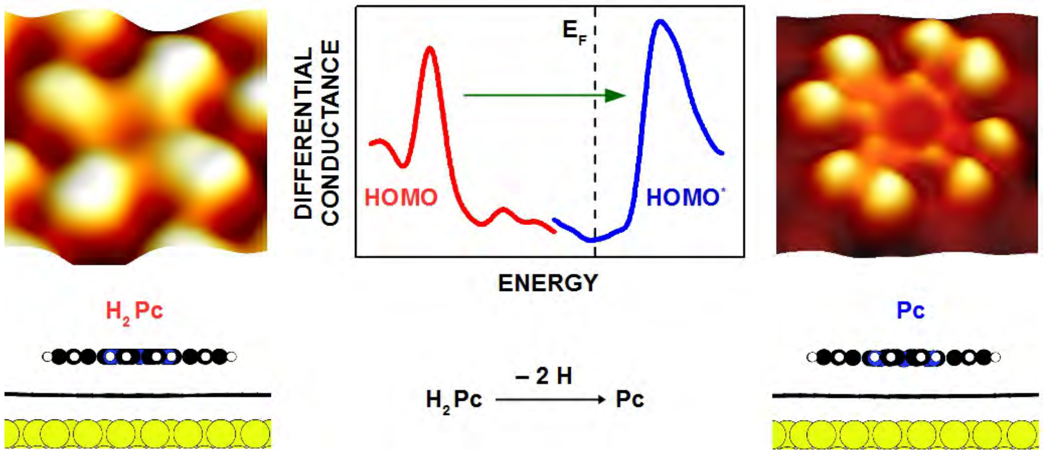
Single-molecule chemistry with a scanning tunneling microscope has preponderantly been performed on metal surfaces. The molecule−metal hybridization, however, is often detrimental to genuine molecular properties and obscures their changes upon chemical reactions. We used graphene on Ir(111) to reduce the coupling between Ir(111) and adsorbed phthalocyanine molecules. By local electron injection from the tip of a scanning tunneling microscope the two pyrrolic H atoms were removed from single phthalocyanines. The detachment of the H atom pair induced a strong modification of the molecular electronic structure, albeit with no change in the adsorption geometry. Spectra and maps of the differential conductance combined with density functional calculations unveiled the entire depopulation of the highest occupied molecular orbital upon H abstraction. Occupied π states of intact molecules are proposed to be emptied via intramolecular electron transfer to dangling σ states of H-free N atoms [1].



Keywords: Single molecule chemistry; Phtalocyanine; Graphene

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INTERACTIONS OF TRANSITION METAL PHTHALOCYANINES AT METAL SURFACES – INFLUENCE OF INTERCALATED GRAPHENE BUFFER LAYERS

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The interactions of molecular layers with substrates strongly influence the charge transport across these interfaces, which may become important for possible future organic electronic and spintronic devices. Here, we report on investigations using X-ray absorption and photoemission spectroscopies (XAS, PES) to elucidate interactions between transition metal phthalocyanines (TMPcs) and metal substrates. In particular, the analysis of TM L-edge spectra (core-level PES and XAS) sheds light on local changes of the interface electronic structure. Valence band and TM L-edge spectra of TMPcs recorded at interfaces on Au(100) point to weak interactions only. But the spectra of the TM central atoms of TMPcs taken on Ag(111) indicate significant interactions including local charge transfer. Similar results were obtained on Ni(111), too [1]. However, for CoPc and FePc on Ni(111) the interactions can be modified by insertion of a graphene buffer-layer [2][3]. MnPc evidently reacts with the Ni(111). Graphene prevents this chemical reaction, reduces the interactions, and suppresses interfacial charge transfer [2][3]. For CoPc on graphene/Ni(111), the prevention of the charge transfer is inhibited by the strong interaction of graphene with Ni(111). This interaction can be weakened or eliminated through intercalation of copper or gold, respectively. Therefore, the disturbance of the graphene electronic structure by the interaction with the metal substrate and the corresponding charge doping has significant impact on the electronic properties of adsorbed CoPc [4].

We gratefully acknowledge cooperations by R. Ovsyannikov, and M. Bauer from Helmholtz Center Berlin, by P. Nagel, M. Merz, and S. Schuppler from ANKA/KIT, Germany, as well by A.B. Preobrajenski and A.V. Generalov, MaxLab, Sweden. We are grateful for financial support from HCB, ANKA, and MaxLab.

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PHOTODEGRADATION OF PCBM AND C_{60} FILMS

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Organic photovoltaics (OPV) may prove to be a competitive alternative to conventional solar cell technologies provided that there is an increase in the stability of large area devices matching what has already been achieved in terms of performance. [1] As a result of efficiency values reaching the threshold for commercial viability, interest in resolving stability and lifetime issues has increased significantly. [2]

Recent studies have focused attention on the degradation of the electron acceptor in solar cells, showing how it can impact strongly on photovoltaic performance and on the long-term integrity of the active layer. [3] Elucidating the mechanisms for degradation in fullerenes and fullerene-derivatives used in solar cells and establishing design rules for the development of more stable acceptors will contribute to increasing the general stability of the devices.

We have studied the photostability of spin-coated PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) and evaporated C_{60} films using photoelectron spectroscopy (PES) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. After exposing these materials in ambient air to simulated sunlight, the filled and empty molecular orbitals are strongly altered, indicating that the conjugated π-system of the C_{60}-cage has been compromised. [4] Studying light-exposed C_{60} films under controlled oxygen- and/or water-atmospheres will aid in elucidating the underlying mechanisms of degradation, pin-pointing the conditions under which they occur.

These results emphasize the need to control processing conditions during OPV fabrication, operation, and storage, while having important implications to the development of high throughput processing strategies.

Keywords: Degradation; Fullerene; Photostability, Photovoltaics.

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COATING CONTAINING MG-DOPED HYDROXYAPATITE PRODUCED BY PLASMA ELECTROLYTIC OXIDATION

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The Plasma Electrolytic Oxidations (PEO) has been used to produce coatings on titanium and its alloys containing high content of HA. The PEO is an electrolytic process carried out with high voltage, in the order of hundreds of volts. The high electric field around the sample generates micro-arcs on coating surface, which produces coating with unique proprieties.

In the present study has been produced coatings on grade 4 titanium with samples of 8 mm diameter and 2 mm thick. The treatment was conducted in a tank capable of storing 1.0 L of electrolytic solution containing 0.2 M calcium acetate, 0.02 M sodium glycerophosphate and magnesium acetate with quantities variables. Between electrodes immersed in the electrolytic solution was applied to anode positive pulses of 480 V with 60% duty cycle and in the cathode, the tank itself, negative pulses of 100 V to cycles of 20% duty cicle, both at frequency of 100 Hz. The treatment time of the samples were 120 s.

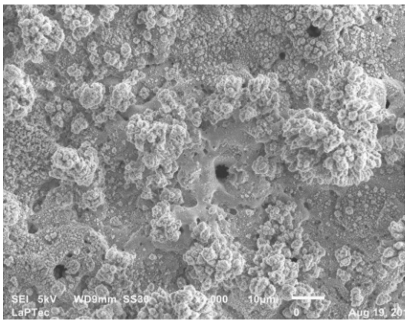

Fig. 1. Coating surface of sample with Mg-doped hydroxyapatite

The coating has been evaluated by profilometry, scanning electron microscopy and X-ray diffraction with Rietveld refinement. The coating composition was evaluated by Rutherford backscattering spectrometry and energy dispersive spectroscopy. The coatings has 50% of Mg-doped HA with incorporation of up to 3.6 a% of Mg, but larger amount of Mg in the solution has produced HA with magnesium phosphate. The effect of doping has been verified by changing the lattice parameters of the crystalline structure of the HA, where the Ca was replaced by Mg

Keywords: Plasma electrolytic Oxidations, Hydroxyapatite, Mg-doped hydroxyapatite

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Modifying diamond substrates by the control of surface oxygen composition.

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The electronic properties and reactivity of surfaces can be significantly varied by changing the nature and quantity of surface adsorbates. This is strikingly demonstrated for the low index faces of diamond where the electron affinity can be changed by several eV from negative to positive by changing the surface termination[1]. This provides a route for engineering surfaces and interfaces for electron emission, electron transport and chemical sensors.

Here, we report a protocol for the oxidation of diamond surfaces and the controlled replacement of oxygen by hydrogen. The latter process has been continuously monitored by real-time electron spectroscopy as illustrated for the O1s core level emission in Figure 1. The fully oxygen-terminated surface at 23ºC is stable up to a temperature of 350ºC (region 1). Above this temperature, the oxygen desorbs rapidly (region 2) and is eventually replaced by hydrogen.

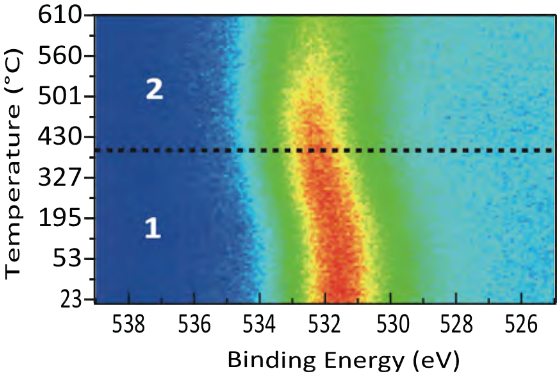

Fig. 1. O1s core level evolution during thermal desorption of oxygen from the diamond (001) surface

Variations in the energy positions of key features in the photo-electron distribution enable compositional changes to be correlated with the electronic structure and chemical reactivity[2]. Control of the surface conductivity is illustrated by adsorbing small molecules on differently prepared diamond surfaces and control of the surface reactivity is illustrated by the interaction of diamond with volatile cancer treatment drug molecules.

Keywords: surfaces; diamond; adsorbates

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IN-SITU STUDY OF THE FIRST STEP'S OF COPPER OXIDE FORMATION ON Cu (110) ELECTRODE SURFACE

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Copper corrosion and oxidation as well as oxygen adsorption process on single crystal copper surface in UHV has been studied systematically [1], However, due to the complexity of the solid-liquid interface [2], the mechanism of the first steps of copper oxide formation in electrochemical environment are not completely understood.

In this work, we study the anodic oxidation of Cu (110) single crystal in 3mM $HClO_4$, PH< 3 acidic solution with Cyclic Voltammetry (CV), in which the integrated charge and ion-exchange is measured. Additionally, we used highly surface-sensitive in-situ Reflection Anisotropy Spectros-copy (RAS) to monitor the reaction processes based on the specific optical respond of the oxide adlayer. The composition of the layers has also been studied qualitatively and quantitatively with chemical and surface analytical methods such as X-ray photoelectron spectroscopy (XPS) at emersed sample. As shown in the CV (Fig.1.), oxide adsorption/desorption peaks are present around -550mv/-600mv. The oxidation was then investigated by comparing the XPS measurement at two defined potentials: one before -550mv and another after -550mv, referring to the pristine Cu metal and copper surface after first oxidation step, respectively. The transition of Cu metal to Cu(I) as a Cu_2O formation is confirmed, with the absence of Cu(II). Our first results provide already additional insight into the oxidation of Cu(110) in acidic electrochemical environment.

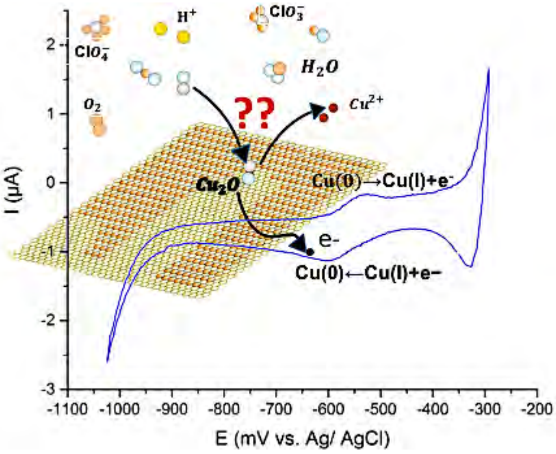

Figure 1. Copper oxide formation on Cu (110) Electrodes in 3mM $HClO_4$

Keywords: Cu (110), XPS, RAS, CV, oxidation, electrochemistry.

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ADSORPTION AND DESORPTION BEHAVIOR OF AN IONIC LIQUID ON ZN-TERMINATED AND O-TERMINATED ZINC OXIDE SURFACES: AN ANGLE-RESOLVED PHOTOEMISSION STUDY

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Ionic liquids (ILs) are salts composed solely of ions that are held together by a strong Coulomb potential. They are generally liquid below 100°C, and many are liquid at room temperature. They have very low vapor pressures, and unlike conventional liquids, can be studied in ultra-high vacuum conditions. They are currently being investigated for a wide variety of applications, including CO_2 capture and storage, corrosion protection, lubricants, and as electrolytes in batteries and photovoltaic devices [1].

For their use in photovoltaic devices, the interface between the IL and the oxide layer (TiO_2 or ZnO) is important. It has recently been shown that ILs can improve the efficiency of ZnO-based polymer LEDs and solar cells by improved charge transport. More specifically, the polarization induced by the ionic dipole is able to reduce the barrier to electron injection between the ZnO layer and the polymer layer [2]. ILs have also shown strong interfacial layering on charged surfaces, as seen in X-ray reflectivity studies of ILs on a charged sapphire (0001) surface [3].

In this work, the interaction of the IL, 1-butyl-3-methylimidazolium tetrafluoroborate ($[C_4C_1Im][BF_4]$), with Zn-terminated (0001) and O-terminated (000-1) ZnO surfaces was investigated using angle-resolved photoemission. Sub-monolayer to multilayer coverages of the IL were vapor-deposited onto the ZnO surfaces both at room temperature and at -150°C. In the latter, photoemission measurements were recorded as the sample was then heated through the IL glass transition temperature, and through to 250°C. Differences in behavior were observed between the two polar surfaces, and the IL was found to reorder as it was heated through its glass transition temperature. In addition, it was found that the IL reacts with the ZnO surface and an anneal was required to remove the reaction products from the surface.

Keywords: Ionic liquid; Photoemission; Photovoltaics; Polar surfaces; Zinc oxide;

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CORROSSION RESISTANCE OF CARBON STEEL COATED WITH A SiO_X-ORGANOSILICON LAYER

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Carbon steel is the most commonly used material for sheets, plates, bars and tubes in mechanical metallurgy and construction industry. However, the susceptibility of carbon steel to oxidation under real conditions of use turns preventive and corrective repairs mandatory. A way to avoid this phenomenon is to coat the metal with a layer, which inhibits permeation of corrosive agents to the metal interface. Some works suggest the development of protective coatings using the plasma deposition technique based on hexamethyldisiloxane, HMDSO, compound. Altering the plasma excitation parameters, enables to deposit organosilicon ($SiO_xC_yH_z$) to oxide (SiO_x) films. Literature works use this flexibility to prepare multilayered films. However most of these works does not study the interference of the order of the layers application on the corrosion resistance of the system. Considering that, the present work aims to study the corrosion resistance of the carbon steel coated with multilayers constituted of SiO_x and $SiO_xC_yH_z$ films in different sequences. SiO_x-organosilicon multilayers were deposited by low pressure radiofrequency (13.56 MHz) plasmas using HMDSO, Ar and O_2 mixtures. The change of an organosilicon to inorganic coating or vice versa was made only by adjusting the plasma conditions without interrupting the process. It was investigated what sequence of monolayers leads to better barrier properties. Electrochemical Impedance Spectroscopy, EIS, and potentiodynamic polarization were used to evaluate the corrosion resistance provided by the multilayer to the carbon steel. Infrared spectroscopy, FTIR, was applied to analyze the chemical composition and molecular structure of the layers. The thickness of the films was measured by profilometry while the morphology and roughness were determined by atomic force microscopy, AFM. The surface wettability was evaluated by contact angle measurements. The best results of corrosion resistance, R_t, of the multilayer system have been obtained with an outermost organosilicon layer. The coating of carbon steel with the multilayered film resulted in an increase of 6 orders of magnitude in R_t.

Keywords: Carbon steel; Corrosion resistance; SiO_x-organosilicon multilayers; Plasma

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SURFACE TRANSPORT ON THIN SEMI-METALLIC FILMS: THE ROLE OF FILM THICKNESS AND MAGNETIC IMPURITIES

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The semi-metal bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentrations and high carrier mobilities. Thereby, epitaxial growth of high-quality thin films opens new pathways to tailor the electronic properties further, e.g. by quantum confinement [1] and alloy formation [2], giving rise to topologically non-trivial states in this material class. In this study we concentrate on Bi films grown on Si(111). Thin Bi(111) films become semiconducting, thus the peculiar spin texture of the surface states, induced by the Rashba effect, can be studied directly by temperature and magnetic field dependent transport.
The conductance G at low temperature is mainly governed by surface states while at higher temperatures activated transport from bulk channels sets it. We have carefully analyzed the G(T)-behaviour for variously thick films. With decreasing film thickness, the bulk gap increases, as expected due to the quantum size effect. However for thinner films the gap decreases and finally the surface states overlap with bulk bands. The reason is an interface-interface interaction which renormalizes strongly the Fermi surfaces [1].
Moreover, magnetic impurities Cr, Co, Fe and Mn, in the range of a few percent of a monolayer were added to probe the scattering behavior of the spin-polarized surface channels by magneto-conductance. The adsorption of all of these elements is accompanied by charge transfer (0.3-0.5h/atom) and strong spin-orbit scattering, which results in a transition of strong weak anti-localization to weak localization. The strength of spin orbit scattering differs among the magnetic atoms and is directly connected to their magnetic moment in the adsorbed state [3].

*Keywords:*semi-metallic films, surface transport, magnetic impurities

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OPTICAL PROPERTIES OF SELF-ORGANIZED NANOSTRUCTURED HYBRIDE FILMS DOPED BY RHODAMINE 6G

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Nanostructured SiO_2 and TiO_2 films were prepared via the template sol-gel pre-doping technique using tetraethoxysilane or titanium isopropoxide as precursor material and Pluronic 123 as surfactant. Dye Rhodamine 6G in different concentration was used as the dopant. It was demonstrated that the method of deposition as well as the condensation rate of the precursor and the evaporation of the solvent reflects in the resulting complexation of the dye. The ability of the occluded Pluronic P123 mesostructures to solubilize organic molecules made these films ideal host matrices for organic dyes and molecular assemblies.

The scheme of the self-organization of the resulting film is shown in Fig.1. Creation of such a columnar structure is directly confirmed by the results of ellipsometric measurements.

Different approaches to the preparation of such a films allow to manage the complexation and optical properties of organic dyes impregnated into the nanoporous silica skeleton. Controlling the Pluronic P123 concentration we are able to control the aggregation of Rhodamine molecules and in such a way to manage fluorescent properties of resulted films [1]. Additionally, optical properties are affected by the geometrical restriction of the aggregation and complexation of organic dyes by the structure of nanoporous silica skeleton. It was demonstrated earlier, that such films have high nonlinear properties and the potential in the use as the photonic layer in an all-optical switching device [2].

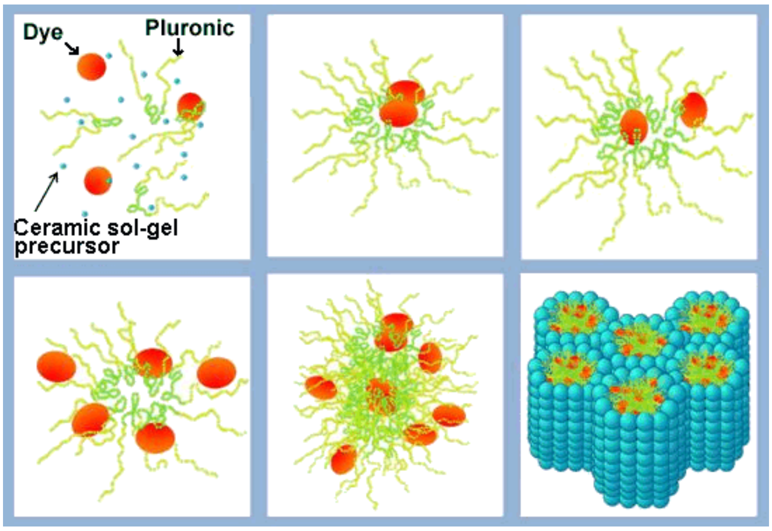

Fig. 1.Self-organization of the film structure

Keywords: Rodamine 6G, self-organization, fluorescence, ellipsometry

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SELECTIVE NUCLEATION OF MnSb ISLANDS ON GaAs SUBSTRATES

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For future spintronic semiconductor devices, spin polarization and injection is one important prerequisite. Ferromagnetic or half-metallic materials are one possible approach for efficient spin-injectors. As with the underlying semiconductor quantum dots, it is necessary to be able to grow the spin-injector material site-selectively in order to build well-defined quantum devices. For site-selective growth of semiconductor quantum dots, two methods were mainly used, which use substrate pre-structuring and surface strain as driving force, respectively. These methods can be transferred to spin-injector materials.

Prestructuring the substrates introduces defects to the surface and may deteriorate the quality of subsequent island growth, which will influence the magnetic properties and lower the spin polarization efficiency. Examples of growth on a prestructured substrate are shown.

Strain-driven nucleation, on the other hand, opens the prospect of pin-pointing exactly one spin-injector island to one semiconductor QD by using the inherent strain induced by the underlying semiconductor QD, so spin-injection can be studied for each QD, individually.

MnSb is an interesting material for spin-injection with its high Curie temperature of 587 K and its compatibility with semiconductor substrates. The strain induced pairing of MnSb islands with InAs QDs is studied. As a first step, structural properties, such as island density and size, have to be matched with the underlying pattern of semiconductor QDs. MnSb islands were grown on different GaAs substrates by MBE. Structural and magnetic properties have been studied by STM, LEED and MOKE.

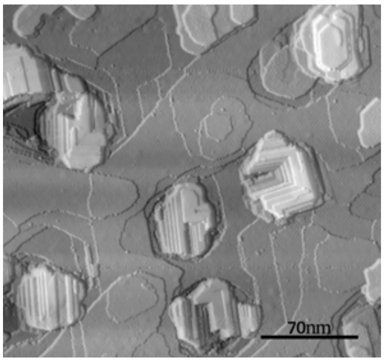

Fig. 1. Example of site-selective growth driven by prestructured substrate. Nucleation of Sb-islands in etch-pits of the GaAs substrate.

Keywords: magnetic nanostructures; Quantum dots; self organized nucleation; GaAs

RAMAN SPECTROSCOPY OF THE LATTICE DYNAMICS AND CRYSTAL FIELD SPLITTING IN $CePt_5$ LAYERS ON Pt(111)

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Ultrathin layers of the binary intermetallic compound $CePt_5$ with thicknesses of few unit cells have found great interest in the field of Kondo physics, originating from the interaction of the localized Ce $4f^1$ electrons with the itinerant electrons [1]. Such $CePt_5$ layers are generated on Pt(111) surfaces in UHV by deposition of elemental Ce and subsequent annealing, resulting in a hexagonal crystalline $CePt_5$ structure, which consists of alternating $CePt_2$ and Pt atomic layers (the latter forming a kagome lattice), and is terminated at the surface by a dense hexagonal Pt layer [2,3]. In this crystal structure a splitting of the Ce 4f electron levels by the crystal electric fields of the neighboring Pt atoms is expected to enable transitions of the 4f electron in the meV range. These transitions should be observable in Raman spectroscopy. Furthermore, the $CePt_5$-layer should give rise to phononic Raman scattering from the lattice.

We report on the determination of the crystal-field-induced 4f level splitting in $CePt_5$ layers with thicknesses between 3.5 and 18 unit cells on Pt(111) surfaces by electronic Raman spectroscopy from crystal field excitations (CFE). For reference we used identically prepared $LaPt_5$ layers, i.e., with the same crystal structure, but without 4f electrons.

In the Raman spectra of $CePt_5$ at $T \approx 20$ K three distinct peaks appear, which are absent for $LaPt_5$. The Raman shifts of these $CePt_5$ peaks range from approximately 15 meV to about 25 meV. Based on the individual dependence of their intensities on the layer thickness, we assign these three peaks to CFE of Ce 4f electrons, located (i) in the $CePt_5$ layer, (ii) at the interface of the $CePt_5$ layer to the Pt(111) substrate, and (iii) at the Pt-terminated surface of the $CePt_5$ layer, respectively.

Besides, up to three additional sharp Raman peaks occur in an almost identical pattern both for $CePt_5$ and for $LaPt_5$. Therefore they are identified as crystal lattice vibrations. For the case of $CePt_5$, one of them is assigned to the $CePt_5$ E_{2g} mode, whose symmetry corresponds to the CFE, the others to vibrations of the uppermost part of the $CePt_5$ layer, which is symmetry-reduced due to surface relaxation [3].

Keywords: Raman; $CePt_5$; Crystal Field Excitations

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MAGNETISN OF Fe3Si FILMS AND ITS CORRELATION WITH ITS CRYSTALLOGRAPHIC PROPERTIES

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The increasing interest in spintronic have motivated the study and development of new ferromagnetic films. Fe3Si is a good candidate as a ferromagnetic electrode due to its high spin polarization and high Curie temperature [1]. Moreover, Fe3Si presents larger resistance when compared to conventional ferromagnets as Fe or Co, which have been proposed as a possible solution for the impedance-mismatch problem in the spin injection through ferromagnet/semiconductor barriers [2, 3]. It is found that the spin-polarized conductance and bias-dependent TMR ratios are rather sensitive to the structure of the Fe3Si electrode. Theoretical studies suggests that there is no spin-polarization for the cubic Fe3Si while, in contrast, the tetragonal Fe3Si presents half-metal nature [4]. Growing thin films allow us to manipulate the structural characteristic of the electrode.

In this context we have prepared by PLD a set of four samples with different crystallographic structure. Fe3Si was evaporated on MgO, STO, LaAlO3 and SiO2/Si getting different crystallographic properties. Clear different magnetic response was obtenied as a function of the crystalograpic behaviour as shown in Fig 1. In this work we will present a complete characterization of the crystallographic structure, elemental composition and magnetism of the samples by RHEED, synchrotron radiation-XRD, XPS and MOKE.

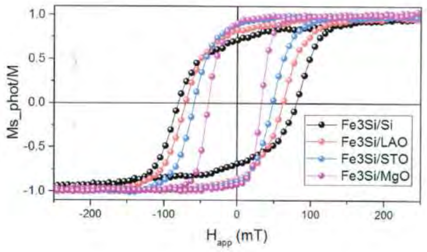

Fig.1: In-plane magnetic hysteresis loops

Keywords: Magnetism; Spintronics

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Structure and bonding control in ultrathin iron films

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Thin films of transition metals such as iron can exhibit different structural, electronic and magnetic properties when grown on different substrates and with different thickness[1]. The highest structural quality requires a close epitaxial match with the substrate and control of the growth parameters.

Here we demonstrate the growth of thin films of iron on epitaxially-matched, single-crystal substrates and non-matched polycrystalline metal substrates, monitored in-situ using laboratory-based and synchtroron-based electron methods (Photolectron Spectroscopy (XPS, UPS), Photoelectron Microscopy (PEEM Electron Diffraction (LEED, LEEM).

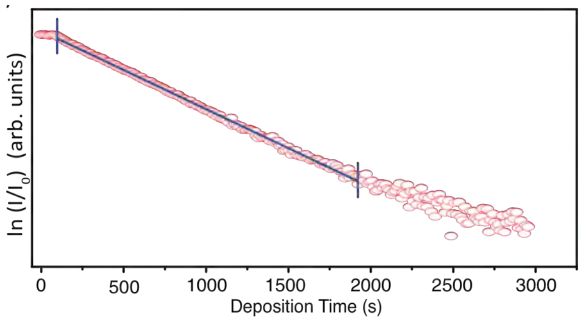

Fig. 1. Real-time monitoring of substrate photoelectron emission during MBE growth of iron.

Epitaxial iron films grown on lattice-matched substrates exhibit 2d growth as shown in the real-time photoelectron emission data presented in Fig. 1. The substrate in this example was a single-crystal diamond, with (111) surface orientation[2]. The C1s core level emission intensity was found to decrease exponentially during film growth, and was fully attenuated by a film of thickness 10 nm. On annealing in vacuum, the FCC iron film exhibited a phase transition to BCC as revealed in LEED and LEEM. Even on non-lattice matched substrates, a change in lattice constant of the iron films was determined from the change in binding energy of the thin film core level states. This was found to correlate with changes in the electronic and magnetic properties of the film.

Keywords: thin films; iron; photoemission

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SURFACE DYNAMICS OF 0.5-1 ML Pb on Cu(111)

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Thin metal films on metal surfaces are of great interest as model systems for materials with reduced dimensionality. For ultra-thin Pb films on Cu(111) it was demonstrated that the HAS inelastic intensities provide a direct measurement of mode-selected electron-phonon (*e- ph*) coupling strengths for individual surface and sub-surface phonons (mode-lambda spectroscopy) [1], thus allowing to assess which phonons are actually relevant in superconductivity. For a correct description of the distribution of the phonon density of states in the film, it is important to take into account the emerging structure of the interface and the interaction between the film atoms and the atoms of the first substrate layer. The calculations presented here are based on the embedded atom method (EAM) and include the dynamics of the substrate (Fig.1). Besides leading to a detailed interpretation of the HAS experimental data, the present results are compared with a density-functional perturbation theory study on a *rigid* substrate. The comparison reveals the role played by the substrate dynamics at the smallest thicknesses, despite the large mass and stiffness differences between Pb and Cu.

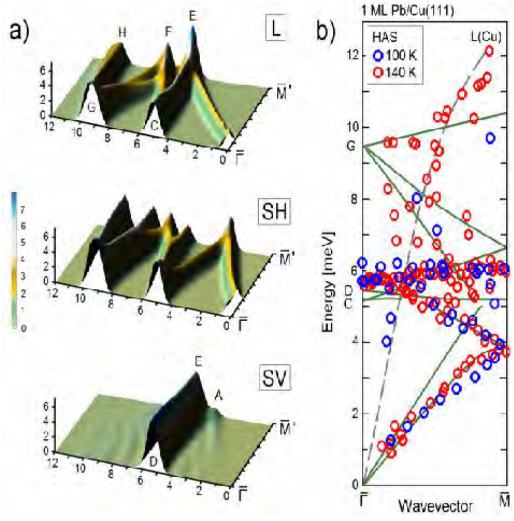

Fig.1. (a) Wave-resolved phonon density and (b) phonon dispersion

The EAM structure analysis also reveals a considerable corrugation of the film surface and of the substrate atomic layers. A dynamically stable structure is formed with a low-energy stretching mode which results from a strong coupling of the monolayer phonons with the low-energy shear-vertical vibrations of the top substrate atoms.

Keywords: Superconducting films, interfaces and surfaces

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PHOTOTHERMAL AND VIBRATIONAL MAPPING OF SURFACES AND INTERFACES BEYOND THE DIFFRACTION LIMIT OF LIGHT

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The diffraction limit of light was regarded as a fundamental unbreakable barrier that prevented the visualization of objects with size smaller than half the light wavelength, until super resolution optical methods and near-field optics allowed overcoming that constraint [1,2]. We report on a new approach based on tracking the photo-thermal expansion (nano-vis) in combination with tip-enhanced Raman spectroscopy (TERS). A commercial TERS system based on atomic force microscopy is coupled to a mechanical switch for intermittent visible light excitation. This simple configuration allows detecting small changes in the nano-object volume. Contrary to nano-IR that is based on the detection of molecular and lattice vibrations [3], the principle behind nano-vis involves tracking the heat generated from electronic transitions and scattering during the relaxation in the sample material that occurs due to optical absorption in the visible spectral range. The sensitivity and spatial resolution are further improved by the combined effect of electric field enhancement obtained by excitation of localized surface plasmons, and the synchronization of mechanical resonance of the tip-cantilever system with the intermittent light excitation. Our concept is demonstrated by the TERS and nano-vis analysis of a two-dimensional material (GaSe) on graphite and by an array of multi-walled carbon nanotubes lithographically designed in a silicon oxide matrix. In addition to TERS, an unprecedented spatial resolution for optical absorption below 10 nm is reported.

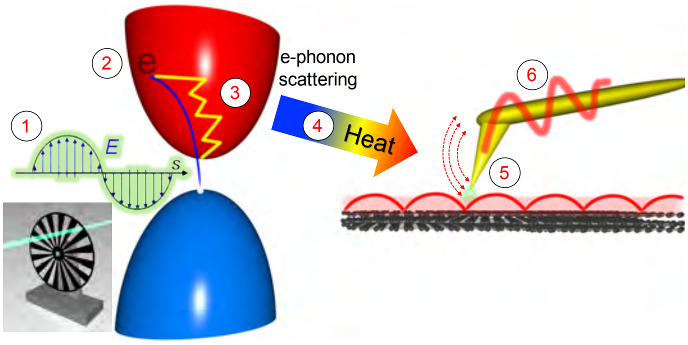

Figure 1: (a) Physical schematics behind nano-vis: (1) a chopper allows the intermittent passage of photons with energy high enough to excite an electron from the valence band to a high energy level (2) in the conduction band, non-radiative relaxation (3) mediated by e-phonon scattering induces (4) heat increase that results in the thermal expansion of the sample (5) and the cantilever deflection (6).

Keywords: nano-optics, photo-thermal imaging, tip-enhanced Raman spectroscopy, TERS, plasmonics, atomic force microscopy

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THE ROLE OF TIP-SAMPLE INTERACTION IN TIP-ENHANCED RAMAN SPECTROSCOPY IMAGING

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The capability to visualize and correlate composition, sample properties, and morphology with a resolution at the nanoscale makes tip-enhanced Raman spectroscopy (TERS) one of the hottest topics in nanoscale characterization since first reported in 2000 [1-3]. Numerical models and previous experimental results showed that the electric field enhancement in TERS is a direct consequence of tip-sample geometry, composition, and laser excitation [4]. In this contribution we show that in addition to those parameters, the tip-sample interaction makes also an impact in image contrast of TERS. Numerical simulations and experimental results show that the attractive tip-sample interaction results in a larger increase of electric field enhancement that is related to an optimal tip-sample distance in that interaction regime. We demonstrate how and why the tip-sample interaction must be considered in the interpretation of TERS imaging results obtained with dynamic mode AFM. These results can be generalized, with implications in other scanning probe based nano-optical methods such as scanning near-field optics (SNOM) with a tuning fork.

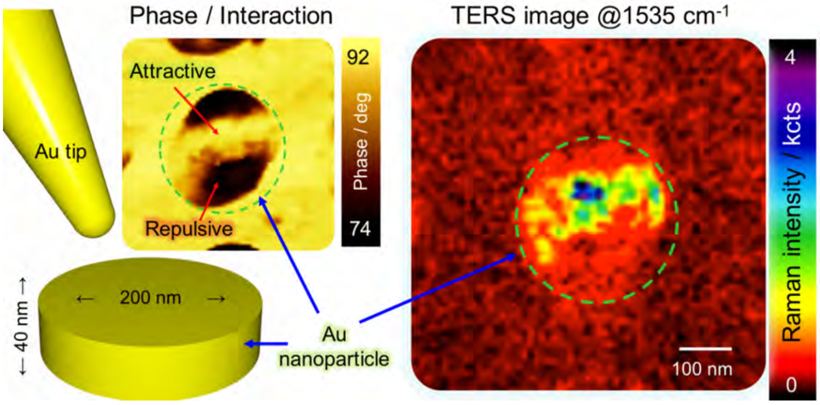

Figure 1: Phase contrast comparison for AFM imaging of a gold nanoparticle with a gold cantilever-tip [5]. The phase image correlation with TERS image contrast obtained under 638 nm excitation, the Raman probe was a 2 nm film of CoPc. The TERS image shows the spatial distribution of the B_{1g} mode intensity of CoPc at 1535 cm^{-1}. Both images were obtained simultaneously.

Keywords: tip-enhanced Raman spectroscopy, TERS, atomic force microscopy, plasmonics

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Ab initio calculations and infrared plasmonic investigation of metallic properties of the Si(111)-(5x2)-Au surface

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Self-assembled atomic wires fabricated on semiconductor surfaces are promising candidates for future nanoelectronics. The Si(111)-(5x2)-Au surface is one of the examples where atomic nanowires appear. For a long time it has been the subject of experimental and theoretical studies. After the revision of the Au coverage to be 0.6 monolayer (ML) [1], new atomic models have been proposed and discussed [2-4]. Erwin *et al.* proposed a model consisting of a gold single row, a gold double row, and a silicon honeycomb chain (EBH model) [2], corresponding to an Au coverage of 0.6 ML. Later, Kwon and Kang proposed a model containing an additional Au atom per (5x2) unit cell (KK model) [3], corresponding to an Au coverage of 0.7 ML. The KK model is energetically favored than the EBH model for rather Au-rich preparation conditions.

The metallic character down to 20 K and the KK model with 0.7 ML Au coverage of the Si(111)-(5x2)-Au surface are confirmed by infrared spectroscopy [5]. Relative transmittance spectra show a broad, anisotropic absorption signal which is attributed to a localized surface plasmon forming a standing wave due to the finite lengths of the wires. The spectral line shape is analyzed quantitatively by a quasistatic absorption cross section which yields important band structure related information. Upon the evaporation of an additional submonolayer amount of gold, the surface becomes insulating but keeps the 5x2 symmetry. This metal-to-insulator transition was in situ monitored based on the infrared plasmonic signal change with coverage [6]. The phase transition is theoretically explained by total-energy and band-structure calculations for a novel structural model.

Keywords: Metallic nanowires; Semiconductor surfaces; Density functional theory; Plasmon

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First-principles calculations of Au-induced wire structures on Ge(001) surfaces: New atomic models for higher Au coverages

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One-dimensional (1D) electronic systems have been investigated extensively because of the interest both in fundamental physics and in nano or atomic scale devices. Self-assembled atomic scale nanowires provide ideal systems for studying peculiar properties of 1D electronic systems. The Au-induced nanowires on Ge(001) are of particular interest in this respect since they are claimed to host a Luttinger liquid [1]. Despite intense research the microscopic atomic structure of Au-induced nanowires on Ge(001) substrates is still under discussion.

We have studied the structural, energetic and electronic properties of Au-induced nanowires on Ge(001) surfaces by means of density functional theory (DFT) calculations studying the p(4x2) but also p(4x4) and c(8x2) translational symmetries [2,3]. We start the investigations from the original [4] and a modified giant missing row (GMR) structure, the Au-trimer stabilized Ge ridge model [5]. Three new structures (shown in Fig. 1) for a higher Au coverage in the range between 1.25 monolayer (ML) and 1.75 ML are proposed and compared with experimental results [2]. Comparing the relative formation energies the new models are shown to be energetically more favorable than the GMR model proposed previously for lower coverages. Indeed, additional Au atoms at the wire surface stabilize novel geometries. The new models are able to explain several features of the nanowire structure observed by scanning tunneling microscopy and the electronic states found experimentally by angle-resolved photoemission spectroscopy.

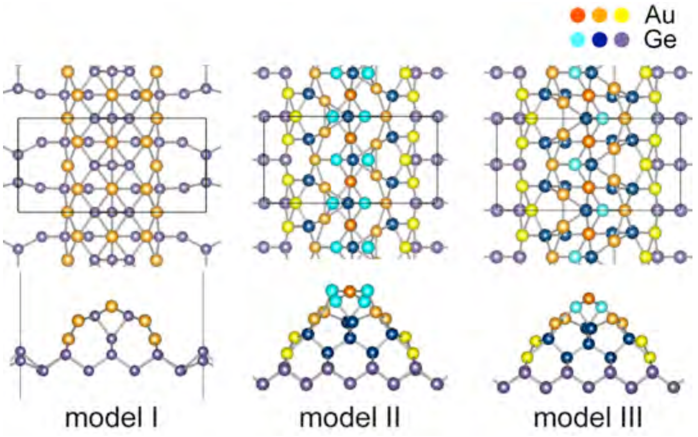

Fig. 1. Proposed structures of the Au/Ge(001) atom chains.

Keywords: Metallic nanowires; Semiconductor surfaces; Density functional theory

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COINCIDENCE LATTICES AND INTERLAYER TWIST FOR OPTIMAL VAN DER WAALS HETEROSTRUCTURES

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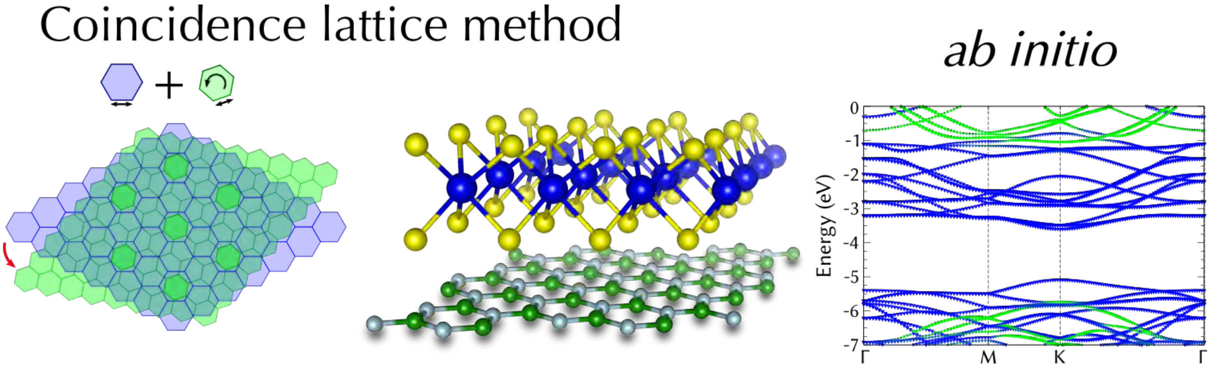

Fig 1: Coincidence lattice method applied on 2D crystals for predictions of vdW heterostructures and *ab initio* calculations.

Van der Waals heterostructures have great potential in large-scale integration devices and new physics exploration. Experimental investigations allow flexible combinations of 2D crystals in device fabrications. Theory, however, has limitations of supercell sizes and commensurability, translated into computational effort. In this work, we demonstrate the application of the coincidence lattice method [1] to simulate two hBN/$MoSe_2$ heterobilayers taking interlayer twist effects into account. We predict that both systems are stable upon contact and interact via van der Waals dispersions. We found that electronic properties of $MoSe_2$ are preserved for both simulated systems, but hBN suffers from the increase of interface interactions, which are evidenced by band structures and density of states calculations. Finally, band discontinuities are obtained and charge transfer arguments explain small shifts in band offsets with respect to natural alignments. We conclude that hBN is a reasonable substrate for maintaining useful properties of $MoSe_2$ for application in electronic and optoelectronic devices and that interlayer twist angles play a significant role in the physics of van der Waals heterostructures.

Keywords: hBN, $MoSe_2$, coincidence lattices method, interlayer twist, vdW heterostructures.

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MODEL DIFFICULTIES FOR PREDICTING THE POLARIZATION SENSITIVE REFLECTED SECOND HARMONIC GENERATION

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In a recent paper from our laboratory we presented the measured second harmonic generation (SHG) response for arbitrarily oriented linear input polarization on Si(111) surfaces in rotational anisotropy experiments[1]. Despite the silicon bulk does not contribute via a dipole transition to SHG, the measured polarization dependent experimental data can only be explained by coherently summing the dipole allowed surface and the quadrupolar bulk SHG sources.

In this contribution we explain the major electrodynamic model aspects for predicting the polarization and intensity response – for clarity we list them with bullet points:

1. First we calculate the strength and direction of the fundamental macroscopic electric field in the material by employing Fresnel's and Snell's laws.

2. The second harmonic polarizability induced ***by the surface dipole*** (C_{3V}-symmetry) can then be calculated by $P_i^s(2\omega) = \varepsilon_0 \sum_{j,k} \chi_{ijk}^{(D)} E_j(\omega) E_k(\omega)$ using a 3rd rank tensor.

3. The second harmonic polarizability induced ***by the bulk quadrupole*** (O_h^7, at any bulk position) can be calculated by $P_i^b(2\omega) = \varepsilon_0 \sum_{j,k,l} \chi_{ijkl}^{(Q)} E_j(\omega) \nabla_k E_l(\omega)$ using a 4th rank tensor.

4. Despite group theory tells that the surface ($\chi_{ijk}^{(D)}$) as well as the bulk tensor ($\chi_{ijkl}^{(Q)}$) have four independent elements, we can analytically prove that for SHG these are reduced to two independent (possibly complex) elements for each of them.

5. In order to handle still less tensor coefficients, we apply the simplified bond hyperpolarizability model (SBHM)[2], which provides for bulk one, for the surface two independent (for one up and three down bonds) tensor coefficients.

6. Because the bulk second harmonic polarization is produced at any depth in the sample and in reflection coherently superimposed at the surface we either fit or analytically calculate (with the given linear dielectric function) the coherent superposition of all bulk waves at the surface. This provides a 4th fit parameter, which can for some physical situations be directly computed.

7. We then discuss the problem of the longitudinal polarizability component, i.e. $\vec{P}(2\omega) \cdot \vec{k}(2\omega) \neq 0$, which occurs for all mentioned tensors at the surface and in the bulk, and how all three polarizability components are transferred to electric ***far-fields*** measurable in the outside by the experimental setup.

8. Finally, we discuss an *ab-initio ansatz*[3] based on density functional theory for predicting the quadrupole contribution of the quantum mechanical response from Bloch functions.

Summarizing, we have implemented steps 1-7 in a forward simulation code and are currently working on a fit program for these 3-4 (complex) parameters.

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AB-INITIO INVESTIGATION OF RARE-EARTH SILICIDE THIN FILMS ON SI(111)

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Rare-earth (RE) silicide thin films grown on silicon surfaces are currently of high interest. They grow nearly defect-free on different surface orientations because of the small lattice mismatch, and exhibit very low Schottky barriers on n-type silicon. Moreover, they give rise to the self-organized formation of RE silicide nanowires on $\mathrm{Si(001)}$ and vicinal surfaces.

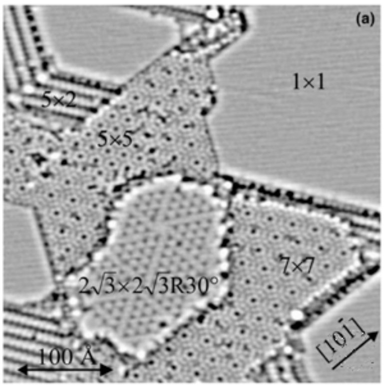

Fig. 1: STM overview images of submonolayer Dy-silicide thin film structures [2].

Depending on the amount of deposited RE atoms, a plethora of silicide reconstructions is observed on the $\mathrm{Si(111)}$ surface. While silicide structures occuring in the submonolayer regime show 5×2 and $2\sqrt{3}\times2\sqrt{3}\,\mathrm{R30°}$ periodicities, one monolayer thick silicides crystallize in a phase with 1×1 periodicity, and several monolayer thick silicides lead to a $\sqrt{3}\times\sqrt{3}\,\mathrm{R30°}$ superstructure.

In this work [1] we investigate the formation of RE silicide thin films on $\mathrm{Si(111)}$ within the density functional theory. We show by ab-initio thermodynamics the occurrence of structures with different periodicity depending on the RE availability and thus reproduce the experimental findings. We calculate structural properties, electronic band structures and compare measured and simulated STM images for each of the silicide phases. Finally, we examine a recent suggestion of a $2\sqrt{3}\times\sqrt{3}\,\mathrm{R30°}$ reconstruction, which is the basis to explain the observation of spot-splitting in SPA-LEED, while STM measurements show no differences compared to the known $\sqrt{3}\times\sqrt{3}\,\mathrm{R30°}$ reconstruction. The calculations are performed with Dy as prototypical RE, but can be extended to other rare-earth elements because of their chemical similarities.

Keywords: Rare Earth Silicide, Si(111), DFT

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TOWARDS EFFICIENT PLASMONIC EXCITATION OF METAL NANO-ANTENNAS AS AN EFFECTIVE TOOL FOR TIP-ENHANCED RAMAN SPECTROSCOPY

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Optical nano-antennas exploit the unique properties of metal nanostructures to increase the efficiency of light-matter interaction in important applications such as nanospectroscopy [1]. They may act as near-field optical probe interacting locally with a sample surface due to its ability to focus light at the nanometer scale for imaging beyond the diffraction limit of light *e.g.* in tip-enhanced Raman spectroscopy (TERS) [2, 3]. Efficient excitation of these plasmon-active noble metal probes is a beneficiary factor to boost TERS performance that we report in this work. We implement an efficient local excitation of plasmons selectively at the probe apex by destructive interference in a patterned SiO_2/Si substrate. As a result we determine the resonance conditions for localized surface plasmons (LSPs) by plasmon modulated photoluminescence (PL) [4]. In the second part of this work we report a significant Raman signal enhancement from the substrate as a result of interference-enhanced Raman spectroscopy (IERS) [5]. Additionally, the sample structure allows to reconstruct the geometry and radius of the probe that gives an all in one ultimate and effective method to design tips for nanospectroscopy and tip-enhanced nano-optics.

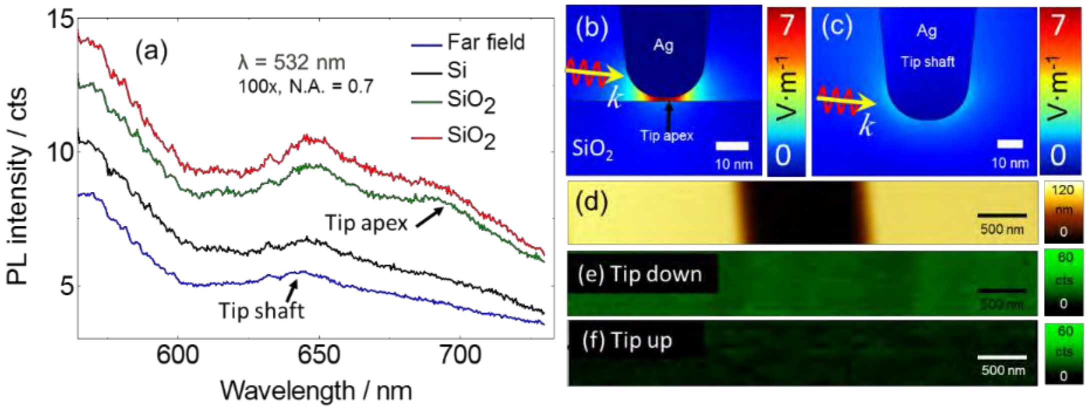

Figure 1: Left: (a) Photoluminescence background for a gold tip above SiO2/Si and without substrate (far field). Right: (b) FEM simulations for spatial distribution of electric field of gold (Au) tips in contact with sample and (c) not in contact with the substrate, (d) AFM topography of the SiO2/Si sample, (e) and (f) TERS images of the Si intensity (at 520.7 cm^{-1}) for tip up and tip down shown at the bottom.

Keywords: Tip-enhanced Raman spectroscopy, interference-enhanced Raman spectroscopy, metal optical nano-antennas, destructive interference.

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HYDROGENATION OF SILICENE PHASES ON Ag(111)

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New elemental two-dimensional materials, such as silicene, are anticipated to show a greater tunability of their electronic properties in contrast to graphene [1]. This is ensured by a higher sensitivity of their properties to structural modifications [2]. For instance, a band gap opening in silicene can be realized by the adsorption of various atomic species, *i.e.* by functionalization [3], or by applying an electric field normal to its lattice [4].

The adsorption of atomic hydrogen on epitaxial silicene on Ag(111) is studied by *in situ* Raman spectroscopy to monitor the structural and electronic modifications upon hydrogenation. The Raman spectra of the hydrogenated silicene give rise to new Raman modes not yet observed, neither for epitaxial silicene nor any other Si allotropes (including polysilanes [7]). Based on the polarization dependence of these modes, which are in agreement with the C_{3v} symmetry of hydrogenated silicene, we determine the approximate patterns of the atomic motion. The hydrogenation was also performed for the different existing phases of epitaxial silicene on Ag(111) exhibiting different Raman spectra. The hydrogenation behavior also depends on the initial silicene phase confirming the results reported in [5,6]. Despite the apparent effect of the hydrogenation on the silicene structure as judged from the Raman spectra and the univocal theoretical predictions of the band gap opening in silicene via hydrogenation, this effect cannot be unambiguously proved by our study, particularly since no photoluminescence was observed. This can be explained by the interaction with the underlying substrate due to either hybridization of the electronic states, or charge transfer to the metal. The hydrogenation of epitaxial silicene on Ag(111) is largely reversible. Upon heating to 230°C the Raman modes of the initial epitaxial silicene layer can almost be recovered. This implies a rather weak bonding of the H atoms to the Si lattice and contrasts the concept of covalent bonding. Consequently, the hydrogenation also does not improve the resistivity of epitaxial silicene to oxidation. Possible capping strategies to prevent silicene from oxidation will be discussed.

Keywords: Epitaxial silicene; Raman spectroscopy; Hydrogenation

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Surface Structure of Semicrystalline Naphthalene Diimide-Bithiophene Copolymer Films Studied with Atomic Force Microscopy

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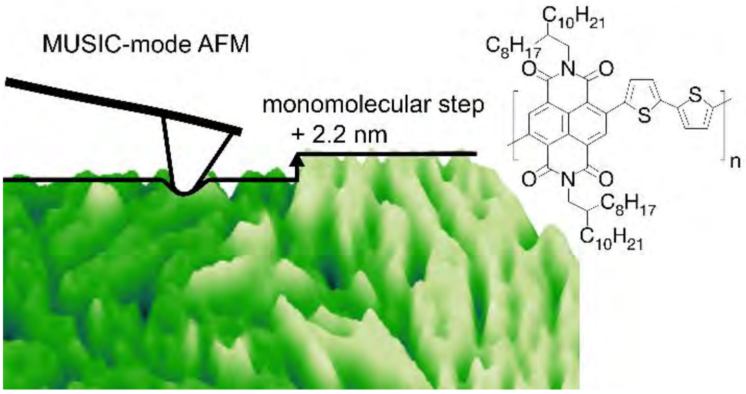
The crystallization behavior, the surface structure, and the nanomechanical properties of a semiconducting polymer play a crucial role in understanding the charge injection process, the transport of the charge carriers, and the processability of the material. Here we study the semiconducting copolymer poly([N,N′-bis(2-octyldodecyl)-11-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5′-(2,2′-12 bithiophene)) (P(NDI2OD-T2)) and investigate the influence of annealing conditions on its surface structure through intermittent contact mode atomic force microscopy (AFM) and AFM-based measurements of amplitude-phase-distance (APD) curves.



For spin-cast thin films as well as for films annealed at temperatures up to 320 °C, we find that the edges of crystalline lamellae are exposed at the surface. A 1.2-nm-thick layer of alkyl side chains covers the film surface as indicated by the tip indentation. This suggests that charge injection into P(NDI2OD-T2) films is not hindered by a surface layer of amorphous material.

In 5-nm-thick films, corresponding to two monolayers of P(NDI2OD-T2), after annealing at 320 °C, crystalline lamella also orient perpendicular to the film plane with the (100) surfaces oriented parallel to the film plane. The lamellae form ~100-nm-large areas (terraces) with uniform lamella height. The step height between adjacent terraces is 2.2 nm, and we attribute it to monomolecular steps between the molecular-thin layers of edge-on-oriented polymer chains. This well-defined molecular conformation at the film surface with the chain backbone and the π-stacking direction oriented in the film plane is presumably an important factor contributing to the exceptional performance of P(NDI2OD-T2) in bottom-gate organic field-effect transistors.

Keywords: Naphthalene Diimide Copolymer; Semiconducting Polymers; Nanomechanical Properties; Dynamic Atomic Force Microscopy

ELECTRONIC AND STRUCTURAL PROPERTIES OF FERECRYSTALLINE COMPOUNDS INVESTIGATED BY PHOTOELECTRON SPECTROSCOPY

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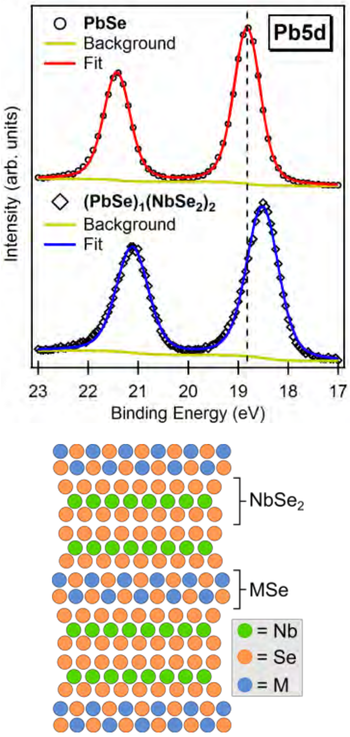

Fig. 1. ***Top:*** XPS Pb5d spectra of a $(PbSe)_1(NbSe_2)_2$ ferecrystal and binary PbSe. ***Bottom:*** Schematic representation of the structure of a $(MSe)_1(NbSe_2)_2$ ferecrystal.

The groundbreaking work on graphene by Novoselov and Geim [1] sparked a run on 2D materials. A combination of different sheet-like materials offers new possibilities in materials properties. The method of *modulated elemental reactants (MER)* [2] enables the preparation of designed turbostratically disordered intergrowths of 2D materials, termed *ferecrystals* [3].

In this work, we investigated the electronic structure of several $(MSe)_1(NbSe_2)_2$ ferecrystals using X-ray photoelectron spectroscopy (XPS). Core level and valence band spectra of ferecrystals with M = Pb or Sn were compared to their respective MER-produced binary compounds MSe and $NbSe_2$. We found evidence of inter-layer interactions and charge transfer as Pb and Sn core levels shift towards lower binding energies in the ferecrystal (Fig. 1).

With XPS, we could also confirm a decrease in the number of antiphase boundaries in $(BiSe)_1(NbSe_2)_n$, when the spacing between the BiSe layers is increased from n = 1 to 2 layers of $NbSe_2$. Antiphase boundaries are a structural modulation occurring in compounds with M = Bi, where Bi-Se bonds are periodically substituted by Bi-Bi bonds [4] (Fig. 2).

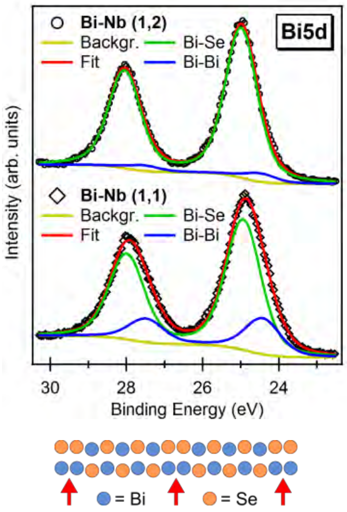

Fig. 2. XPS Bi5d spectra of two $(BiSe)_1(NbSe_2)_n$ ferecrystals with different layer stacking (short Bi-Nb (1,n)). The number of Bi-Bi bonds at antiphase boundaries (red arrows) decreases for n=2.

Keywords: Ferecrystals; Layered Compounds; XPS; Charge Transfer

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Stability of GaSe Monolayers

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Two-dimensional (2D) van der Waals semiconductors have been the subject of intense research due to their ultra-low dimension and tunable optoelectronic properties. GaSe (a typical metal monochalcogenides, MMC; MX: M = Ga, In; X = S, Se, Te) belongs to that class of semiconductors and it is of growing interest owing to its optoelectronic properties. However, monolayer stability of this material is one of the important question that needs to be clarified, especially for technological applications. Drapak *et al*. showed that a layer of native oxide forms on a cleaved surface of a bulk GaSe crystal due to storage in air for prolonged time [1. Very recently, the degradation of optical properties of few nm thick GaSe was reported by Zamudio *et al*. [2] while Beechem *et al*. [3] studied the physical process of degradation in GaSe of thicknesses varying from 4 nm to few hundred nm. But environmental stability of GaSe over time is still remained unknown. Here the time stability of GaSe monolayer was investigated by Raman spectroscopy, X-ray photoemission spectroscopy (XPS), phase imaging in dynamic atomic force microscopy, and surface potential mapping. Raman spectroscopy study shows that GaSe monolayers survive only for 5 hours. After that period, GaSe single-layers decomposed into amorphous Se, which is also a good agreement with XPS results. The surface potential study showed GaSe completely passivated by oxidation after 12 hours. The present study provides a clear picture of the monolayer stability in air and will guide future research of GaSe from single- to few-layers in the developing of novel technological applications.

Keywords: 2D materials, GaSe, monolayer stability, oxidation

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SPECTROSCOPIC ELLIPSOMETRY STUDIES OF $TlIn(S_{1-x}Se_x)_2$ SOLID SOLUTIONS AT DIFFERENT TEMPERATURES

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$TlInS_2$-type crystals are layered ferroelectric semiconductors with a complex sequence of structural phase transformations including incommensurate phase in the interval 201–216 K [1]. Besides, a Lifshitz-type point is possibly observed in the (x, T) phase diagram of $TlIn(S_{1-x}Se_x)_2$ solid solutions at $x = 0.05$ [2].

Here we report on ellipsometry studies for $TlIn(S_{1-x}Se_x)_2$ solid solutions at different temperatures. $TlIn(S_{1-x}Se_x)_2$ ($x = 0$, 0.05, 0.08, 0.25) single crystals were obtained by Bridgman technique. The real ε_1 and imaginary ε_2 parts of the dielectric function of the $TlIn(S_{1-x}Se_x)_2$ single crystals were obtained in the 1 to 5 eV spectral range in the (001) layer plane. Temperature studies of energy dependences of ε_1 and ε_2 in the temperature range 143-293 K were performed using a Linkam stage THMS600.

The measured ε_1 and ε_2 spectra exhibit several optical features associated with interband transition critical points (CPs). Their energies were determined by analyzing the calculated second-energy derivatives of functions obtained from the ellipsometric measurements.

Analysis of the second derivative spectra of the dielectric function at room temperature in the above-bandgap region revealed the presence of four critical points at $E_{c1} = 3.24 \pm 0.01$ eV, $E_{c2} = 3.33 \pm 0{,}01$ eV, $E_{c3} = 3.59 \pm 0.01$ eV and $E_{c4} = 4.52 \pm 0.05$ eV for $TlInS_2$, five critical points at $E_{c1} = (3.24\pm0.01)$ eV, $E_{c2} = (3.32\pm0.02)$ eV, $E_{c3} =(3.60\pm0.01)$ eV, $E_{c4} = (4.25\pm0.1)$ eV, and $E_{c5} = (4.39\pm0.1)$ eV for $TlIn(S_{0.95}Se_{0.05})_2$, $E_{c1} = (3.25\pm0.01)$ eV, $E_{c2} = (3.30\pm0.02)$ eV, $E_{c3} =(3.61\pm0.01)$ eV, $E_{c4} = (4.27\pm0.3)$ eV, and $E_{c5} = (4.36\pm0.3)$ eV for $TlIn(S_{0.92}Se_{0.08})_2$ as well as six critical points at $E_{c1} = (2.68\pm0.01)$ eV, $E_{c2} = (2.88\pm0.05)$ eV, $E_{c3} = (3.49\pm0.5)$ eV, $E_{c4} = (3.51\pm0.5)$ eV, $E_{c5} = (3.65\pm0.2)$ eV, and $E_{c6} = (4.31\pm0.2)$ eV for $TlIn(S_{0.75}Se_{0.25})_2$ crystal.

Temperature dependences of interband transition energies for $TlIn(S_{1-x}Se_x)_2$ crystals are discussed.

Keywords: ferroelectric; dielectric function; critical point

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BRIGHTLY LUMINESCENT COLLOIDAL Ag-In-S NANOPARTICLES STABILIZED IN AQUEOUS SOLUTIONS BY BRANCHED POLYETHYLENEIMINE

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A direct and mild synthesis of water-soluble brightly luminescent Ag-In-S nanoparticles (NPs) stabilized by branched polyethyleneimine (PEI) is proposed. The key parameters influencing spectral parameters and photoluminescence (PL) intensity of Ag-In-S NPs are (i) the Ag:In and Ag:S ratios and (ii) duration of the post-synthesis thermal treatment of colloidal solutions at ~100 °C. A variation of the Ag:In ratio allows to tune the PL color from green to orange-red (Fig. 1). The maximal PL quantum yield, 20%, was observed for the Ag-In-S-PEI NPs produced at a molar Ag:In:S ratio of 1:5:5 and 2-h post-synthesis thermal treatment at around 100 °C. Dynamic light scattering showed that such NPs have an average hydrodynamic size of ~100 nm. According to SEM each 100-nm globule comprises many separate smaller Ag-In-S NPs. Reasonably high PL quantum yield, variability of the emission color and self-aggregation of Ag-In-S-PEI NPs into polymer globules that do not scatter light makes such NPs promising for the luminescent bio-labeling applications. The PL band maximum energy of the Ag-In-S-PEI NPs produced in optimal conditions is very close to the band gap derived from the absorption spectra of colloidal solutions indicating that the PL originates either from the radiative recombination between delocalized conduction band electron and valence band hole or from the radiative recombination with the participation of the charge carriers captured by “shallow” traps. A large spectral width of the PL bands of Ag-In-S-PEI NPs can be interpreted as a result of size distribution of NPs residing in a regime of strong spatial exciton confinement.

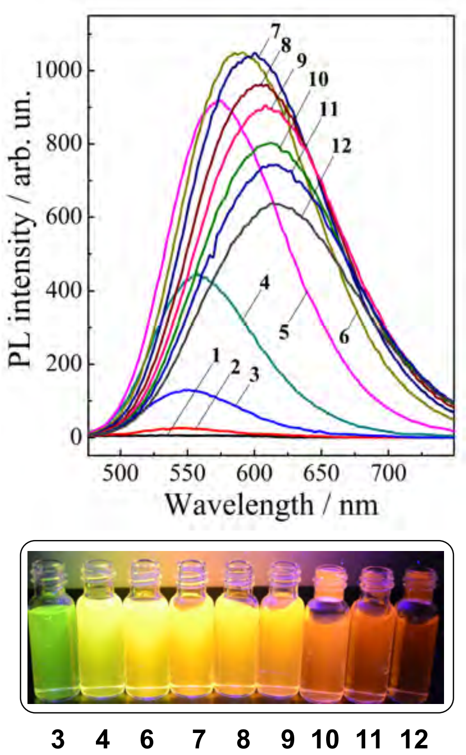

Fig. 1. PL spectra and photographs of colloidal Ag-In-S NPs synthesized at Ag:In:S ratio = x:5:5, x = 0.1 (curve 1), 0.2 (2), 0.3 (3), 0.5 (4), 0.7(5), 0.9 (6), 1.0 (7), 1.1 (8), 1.2 (9), 1.3 (10), 1.4 (11), and 1.5 (12). PL was excited at λ = 450 nm. Photographs were taken under UV illumination (350-400 nm).

The work is supported by the Volkswagen Foundation (project “New functionalities of semiconductor nanocrystals by controllable coupling to molecules”).

TEMPERATURE DEPENDENT EXCITON-PHONON COUPLING IN SEMICONDUCTOR CdSe/ZnS QUANTUM DOTS

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One long standing question in semiconductor quantum dots (QDs) physics is the effect of quantum confinement on the strength of exciton-phonon coupling (EPC) and phonon frequency, a topic that has received considerable experimental and theoretical attention. Upon evaluation of EPC parameters for QDs, the majority of previous temperature experiments have been carried out for QDs dissolved in rigid matrixes (polymers, resins, *etc.*). In this report, we will discuss temperature dependent exciton-phonon coupling in CdSe/ZnS QDs capped by TOPO ligands and embedded into a glass forming liquid. In the later case, a possible phase transition of the capping ligand layer should be taken into account.

While in most reported experiments photoluminescence (PL) data (PL energy; PL band width, or Stokes shifts) have been used to determine EPC parameters we used in parallel temperature dependent absorption data which provided in combination with PL emission the identification of the temperature dependence of the Stokes shift, which in return reveals temperature dependent Huang-Rhys factors. We found that temperature dependent data from absorption are slightly but definitely different from those obtained by PL. We explained this finding by the analysis that absorption is more sensitive to core CdSe LO optical phonons while PL also contains coupling to ZnS phonons of the shell. In addition, as we shown recently [1] PL emission of QD is to a large extent due to QD surface states. A phase transition-type changes were found in absorption and PL. From the temperature dependent Stokes shift analysis it was elucidated that EPC below the phase transition temperature T_{crit} is governed more efficiently by coupling to ZnS phonons, while above coupling to CdSe increases. This result is supported by the observation that the (size dependent) phase transition appears at lower temperatures (≈ -10 K) in absorption (predominant excitation of small QDs) as compared to the one detected in PL from dominantly surface states. It follows from the obtained results that determination of EPC via Stokes shifts needs a temperature dependent investigation to reduce (i) contributions from the thermalization of the excitonic fine structure levels, (ii) influence of differently contributing near-band-edge states and shallow traps and (iii) identification of the “true“ first absorption band. Neglecting these influences will result in too large Stokes shifts and exciton-phonon coupling constants.

Finally, the most interesting finding is that contrary to results reported in literature, temperature activated coupling to optical phonons proceeds not via excitation to the second excitonic state but to a recently identified hole state which has often been overlooked in several reported investigations.

Keywords: Semiconductor quantum dots, Ligand dynamics, Photoluminescence, Absorption, Surface traps, Exciton-phonon coupling, Temperature surface “phase” transition.

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CONFINED AND INTERFACE PHONONS IN 2D COLLOIDAL NANOCRYSTALS

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Recently developed 2D colloidal semiconductor nanocrystals, or nanoplatelets (NPLs) [1], extend the range of solution-processable free-standing nanomaterials of high performance. Growing CdSe and CdS subsequently in either side-by-side or stacked manner results in core-crown or core/shell structures, respectively. Both kinds of hetero-NPLs find efficient applications and represent interesting materials to study the elemental excitations under strong one-directional confinement [2].

Here, we investigated by Raman and infrared spectroscopy the phonon spectra and electron-phonon coupling in CdSe/CdS core/shell and core-crown NPLs. A number of distinct spectral features of the two NPL morphologies are observed, which are further modified by tuning the laser excitation energy E_{exc} between in- and off-resonant conditions. The general difference is the larger number of phonon modes in core/shell NPLs and their spectral shifts with change of shell thickness or E_{exc}. The spectra of the core-crown NPLs are more resembling the sum of spectra of the isolated CdSe and CdS particles, and are similar to spherical morphologies studied earlier. This behaviour is explained by mutual influence of the core and shell in NPLs and formation of combined modes. In the core-crown structure, the CdSe and CdS modes preserve more independent behaviour with only interface modes forming overtones with core phonons.

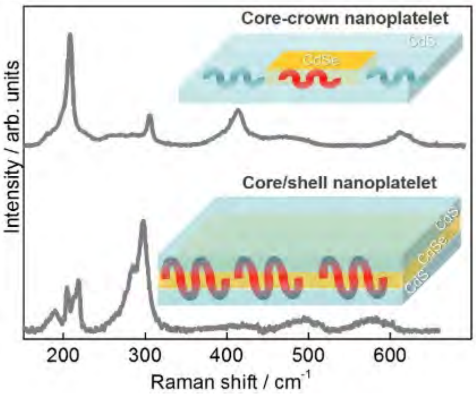

Fig. 1. Representative resonant Raman spectra of two types of CdSe/CdS NPL morphologies shown in the insets.

Keywords: Semiconductor Nanocrystals, Interface, Core-Shell, Phonons, Raman, Infrared

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Solid-phase interaction in the bilayer eutectic nanofilms

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Low-temperature solid-phase interaction in the simple eutectic pairs of metal-semiconductor nanofilms is one of the ways to create new materials for engineering of nanoplasmonic and nanophotonic structures. In present report bilayer systems of semiconductor and metals that are forming simple eutectic pairs Ge-Au, Ag, Al, the changes of structural and optical properties of this bilayer eutectic nanofilms during the laser and thermal annealing were investigated. Bilayer eutectic nanofilm systems were prepared by thermal evaporation in vacuum with computer control technique.

The nanostructure with total thickness 45 - 50 nm and width of pits 0,5mkm was obtained via laser beam treatment of two-layer eutectic system Ge-Au, Ag, Al. The annealing was performed by laser with a wavelength of 530 mkm. The laser annealing power of this structures on glass substrates was 4-11mW [1,2].

The results of bilayer eutectic nanofilms thermal annealing demonstrate the changing of transmission and reflection index. At the same time AFM images of samples before and after the thermal annealing show the same structure. The temperatures of solid-phase interaction of investigating samples was 1,5-3 times less then eutectic temperatures. Spectra of binary mixtures Ge-metals were measured in situ during the thermal annealing. Also be noted that reflection index spectra of the systems Ge-Au,Ag,Al before and after annealing are different [3]. All features of the investigated systems described above can be used for creation photonic crystals.

One of the main elements of the surface plasmon resonance (SPR) technique is SPR biosensor chips (glass plate with 50 nm Au). This paper reports an effective method to enhance the surface plasmon resonance (SPR) on Au films by using a thin Ge layer. Au films with a thickness of about 50 nm were deposited by thermal evaporation in vacuum above an ultrathin Ge layer of ~2 - 5nm on glass substrates. The surface roughness have been reduced from >5 nm for a pure Au film to ≤1nm for Au/Ge films, respectively Our results show that Ge acts as a roughness-diminishing growth layer for the Au film while at the same time maintaining and enhancing the plasmonic properties of the combined annealling structures. This points toward its use for low-loss plasmonic devices and optical metamaterials applications.

Keywords: bilayer eutectic nanofilms, laser and thermal annealing, surface plasmon resonance, metamaterials, gold, germanium,surface roughness.

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VIBRATION EIGENMODES OF THE ORDERED ADSORBATE Au-(5X2)/Si(111): RAMAN SPECTROSCOPY AND FIRST-PRINCIPLE CALCULATIONS

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A sub-monolayer coverage of metal atoms on a semiconductor surface can exhibit a self-assembled reconstruction pattern, inducing electronic correlation effects, especially for one-dimensional chains. These effects are tightly connected with the local arrangement of the atoms and the corresponding vibration eigenmodes. For this purpose, the Au/Si(111) system has found broad interest. Well-defined reconstruction patterns can be induced for appropriate Au coverages and substrate temperatures, e.g. the Au-(5x2) reconstruction, consisting of parallel chains with Au single and double rows. Its vibration eigenfrequencies and mode symmetries can be studied with high spectral resolution by Raman spectroscopy.

We report on polarized *in-situ* UHV Raman spectroscopy of the vibrational eigenmodes of self-assembled Au-structures on Si(111) surfaces, whose (5x2) reconstruction was confirmed by LEED. Although the intensity of the Au- and surface-related Raman signals is about four orders below the Si bulk phonon signal because of their extremely low scattering volume, high-sensitivity CCD detection allows the identification of the Au-induced vibration modes. In the Raman spectrum they replace the peaks which were previously identified as surface vibration modes of the clean (7x7)-reconstructed Si(111) surface [1]. The positions of the Au-induced Raman peaks are in the range between 3 meV and 15 meV, the strongest ones at 3 meV, 6 meV, and 13 meV. These Raman peaks show mode-specific polarization properties, which are strongly correlated with the direction of the Au-induced chains.

Furthermore, we performed first-principles calculations of the Au-(5x2)/Si(111) surface dynamics within Density Functional Theory as implemented in the VASP package. In addition to eigenmodes patterns and eigenfrequencies, we calculated also the Raman scattering efficiencies. This allows the comparison of our experimental results with the calculated vibrations for two currently discussed Au-(5x2) reconstruction models, an intrinsically (5x1) model by Erwin *et al.* [2], which achieves the (5x2) periodicity by invoking a double-periodicity arrangement of Si adatoms along the chains, and alternatively a modified model by Kwon and Kang [3], where one additional Au-atom per unit cell yields a genuine (5x2) periodicity.

Keywords: Au-(5x2)/Si(111), Vibrations, Raman, First-Principle Calculations

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ATOMICALLY FLAT SURFACE RECONSTRUCTION OF THE Bi_2Te_3 TOPOLOGICAL INSULATOR

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Topological insulators (TIs) are materials with an insulating bulk interior and a single, non-degenerate Dirac fermion band on the surface [1]. Of the available TIs bismuth telluride (Bi_2Te_3) has received considerable attention due to its promising applications in spintronics. Bulk Bi_2Te_3 has a layered structure consisting of quintuple layers (QLs) with each QL consisting of a sequence of Te-Bi-Te-Bi-Te atomic planes [2]. This allows for a convenient cleaving between adjacent QLs along the (111) direction. Here, we present the results of our detailed study of the influence of annealing under UHV conditions on surface reconstruction behavior of freshly cleaved Bi_2Te_3. We investigated this surface behavior using UHV scanning tunneling microscopy (STM). We found that there is a gradual change in the surface reconstruction of the Bi_2Te_3 with the annealing temperature (Fig. 1). Additionally, annealing to 400 °C results in an atomically flat surface with an increased density of the atomic steps on the Bi_2Te_3 surface. Moreover, Auger spectroscopy reveals the appearance of a Bi (111) bilayer as the top most layer atop the QLs after annealing at 400 °C, which is further supported by STM height profile measurements. Our systematic investigation may provide a pathway to overcome the difficulties which are associated with complex in-situ surface preparation techniques.

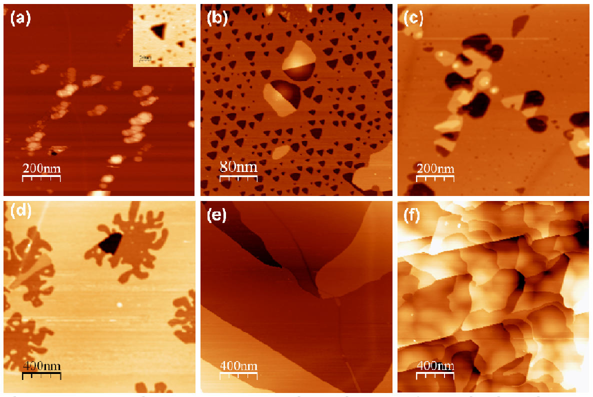

Fig. 1. STM images revealing the surface behavior (a) before the annealing and for different annealing temperatures: (b) 200, (c) 250, (d) 290, (e) 330, and (f) 400 °C under UHV conditions.

Keywords: Bi_2Te_3; Topological Insulator; Scanning Tunneling Microscopy

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CONTROL OF METALS SULFIDE NANOCRYSTALS GROWTH: MORPHOLOGY AND APPLICATIONS

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Nanocrystals of metals sulphide – NiS, AgS, CdS (NC) are very prospective nanoobjects due to crystalline anisotropy, photoconductive, ferroelectric and magnetic properties of material. Control of NC growth from gaze phase give us ability to change morphology from amorphous or polycrystalline nanowires to single crystal nanoobjects. Its diameter may be in the range of tens and hundreds of nanometres and length – from hundreds nanometres to tens of microns. What is why scanning electron microscopy gives us important information on NC morphology. In our experiments NC are grown from gaze phase in the quasi-closed volume. Design feature of NC growth setup gives us ability to stop the growth of NC and reevaporate it partially.

Value of diffusion length can be measured from NC shape if NC had been grooved when transport is a limiting factor in the chain of NC growth stages. In our experiments diffusion length had the order of microns and it can be controlled by saturation and substrate temperature. Nucleation and crystallization rate relation in the vapor-liquid-solid growth determines shape of the nanowire and its crystallinity. Analysis of growth rate as a function of NC diameter allows us to estimate time of crystallization front propagation and time of nucleation. Nucleation time can be found in the range of seconds. If nucleation time is lower than the time of crystallization front propagation then growth of nanosize monocrystal can be realized in monocentric mode. At the polycentric mode probability of nucleation of a few nucleus is enough during the time of crystallization front propagation. Knowledge of diffusion length, nucleation time and crystallization rate as a function of conditions of growth allows us to control crystallinity and morphology of CdS nanocrystals.

Piezoelectric properties of CdS NC give us ability to design piezoresonance sensors with projective sensitivity in order of 10^{-16}g due to small mass of single NC.

The peculiarity of CdS tripode and tetrapode nanocrystal elements is the fact that under certain conditions of heteroepitaxial growth its geometry is determined by the crystallographic structure of semiconductor substrates what governs the orientation of tripods, and only length is defined by the technological parameters of growth kinetics. Application areas of tripode and tetrapode nanocrystal are: nanoantennas - detectors of radiation, electroluminescent devices, biosensors.

Growth of semiconductor nanocrystals in the microelectrodes space is a self-organizing process suitable for one dimensional devices manufacture as opposed to existing technique of single crystal attaching to microelectrodes by micromanipulator and connecting into electric circuit by electron-beam lithography. Our approach to this problem is based on the use of processes of self-organization of semiconductor nanocrystals, which will allow us to grow nanocrystals with a given morphology, crystallinity, type of lattice and to form the complete device. Application of single nanocrystal element is biosensor which consists of microelectrodes and a one-dimensional single semiconductive nano- crystal connected in the electric circuit.

Keywords: nanocrystal, growth, nucleation, crystallization, SEM, morphology, biosensor

Synthesis and Characterisation of Trinuclear Ni_2Cu- and Co_2Cu-Hexaaza-bis(dithiopenolato)-complexes

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The development of dinuclear complexes and the investigation of their magnetic properties have become an attractive prospect in the last few years. In our working group we focus on the preparation of macrocyclic compounds with nitrogen and sulphur donor atoms being capable of forming dinuclear metal complexes. The properties and coordination behaviour of the macrocyclic ligand $\mathbf{H_2L^{Me2H4}}$ has been intensely investigated during the last few years.[1] This ligand supports the formation of mixed-ligand complexes of the type $\mathbf{[M_2(H_2L^{Me2H4})(\mu\text{-}L')]^+}$.[2,3] Due to the free coordination side, the cavitand obtains the ability to act as a molecule sensor for small anions. The bridging coordination site is accessible for spherical and linear anions. We will present the syntheses of dinuclear complexes with hydroxyl and fluoride as spherical coligands with the selected transition metals cobalt and nickel. Than this complexes were additionally bridged over copper(I)-salts at one sulphur atom to the $\mathbf{[M_2(H_2L^{Me2H4})(\mu\text{-}L')(CuX_2)]}$ type.[4] The obtained trinuclear nickel(II/II)-and cobalt(II/III)-complexes with copper(I)-salts were characterised by mass spectrometry, UV/Vis-, IR spectroscopy, molecular structure and temperature dependent magnetic susceptibility measurements.

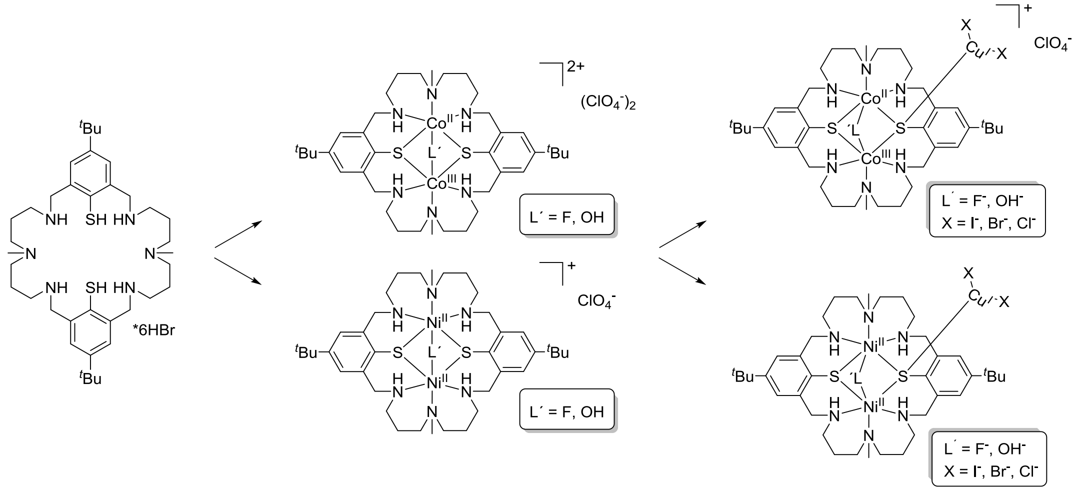

Figure 1. Syntheses of the trinuclear complexes.

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SYNTHESIS, CHARACTERIZATION AND THERMAL STABILITY OF (METALLO)PORPHYRINS

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During the last decades (metallo)porphyrins have been studied in great details as they exhibit a high chemical and thermal stability, as they are aromatic and possess a distinctive electrochemical and photophysical properties[1a,b]. We did already contribute to such studies and reported on deposited thin films using porphyrins of the type **H_2**THPP (tetra(p-hydroxyphenyl)porphyrin[2a,b], cf. Fig. 1, and **M**TMPP/**H_2**TMPP (tetra-(4-methoxyphenyl)porphyrin, (M = Cu[2c], Cu [2d], Ni[2d]).

The properties of the (metallo)porphyrins are governed by the bound (transition) metal ion, exocyclic moieties on the individual pyrrole fragments and/or on the meso positions. Comparative studies of the accessibility and characterization of (metallo)porphyrins are rarely reported in literature[1a, 3], which limits possibilities to select the porphyrin of choice by a knowledge-based approach. Results obtained for two series of porphyrins of the type **H_2**/**M**TPP($CON(R)_2$)$_4$ (series I/II, cf. Fig.1) will be presented with respect to their synthesis and characterization (FT-IR, NMR, UV-Vis, EA, ESI-MS, TGA). Additionally, their molecular and crystal structures determined by single-crystal X-ray diffraction studies will be shown. Based on the thermal stabilities of series I/II porphyrins determined by thermogravimetric analyses (TGA) in comparison with, for example, that of **H_2**THPP, cf. Fig. 1 (right), limits for the thin film fabrication methods will be discussed.

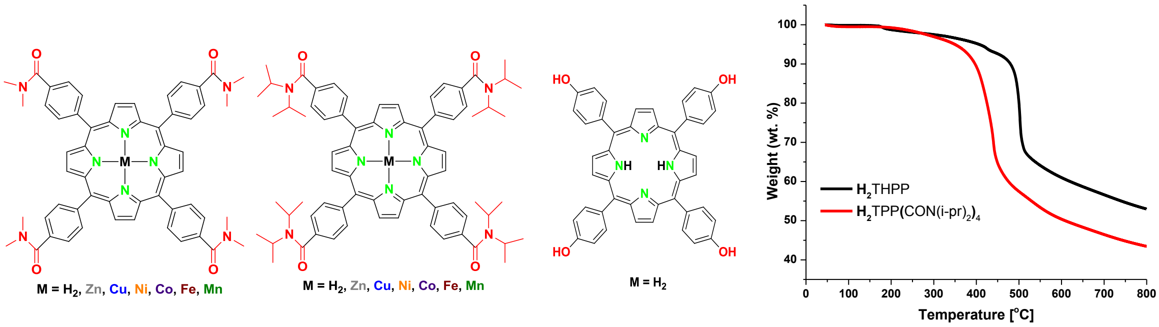

Fig. 1. Chemical structures of **M**TPP($CON(R)_2$)$_4$ porphyrins of series **I** (left) / **II** (middle) and of **H_2**THPP (right). TGA curves of **H_2**THPP and **H_2**TPP(CON(i-Pr)$_2$)$_4$ (right).

Keywords: (metallo)porphyrins, molecular / crystal structure, dispersion interactions, thermal stability.

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Tetranuclear 3*d*-Transition Metal Complexes of a Macrocyclic N_4S_4-Donor Ligand: Synthesis, Characterisation and Magnetic Properties

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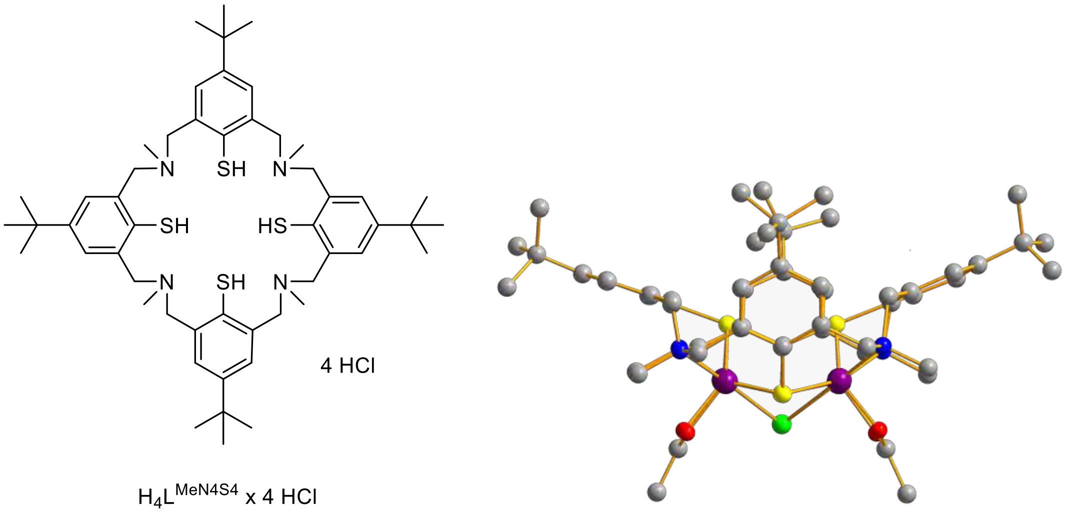
In the last decade much effort has been invested in synthesis and characterisation of polynuclear transition-metal thiolate complexes, due to their intriguing magnetic and electronic properties [1]. In 2014 SCHLEIFE developed a synthesis for a novel amino-thiophenolatoligand, which is able to form tetranuclear complexes [2].



H_4L^{MeN4S4} x 4 HCl

Figure 1. Tetraaza-tetrakis(thiophenolato)-ligand $\mathbf{H_4L^{MeN4S4}}$ (**left**), Molecular structure of Cobalt-benzoate-complex $[Co_4\mathbf{L}^{\mathbf{MeN4S4}}(\mu\text{-Cl})(\mu\text{-OBz})_2]^+$ (**right**) (Co: purple, S: yellow, N: blue, Cl: green).

The syntheses and characterisation of selected tetranuclear 3*d*-transition metal complexes are presented. The magnetic exchange interactions of some complexes are investigated by temperature depending magnetic susceptibility measurements.

Keywords: Macrocyclic Ligands; Magnetochemistry, Tetranuclear Cobalt-complexes

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Electronic structure of novel charge transfer compounds: application of Fermi-Löwdin orbital self-interaction corrected density functional theory

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We present our theoretical results on novel Picene/F_4TCNQ and Manganese-Phthalocyanine/F_4TCNQ donor / acceptor systems. We apply the recently developed Fermi-orbital based approach for self-interaction corrected density functional theory (FLO-SIC DFT) to these materials and compare the results to standard DFT calculations and to experimental data obtained by photoemission spectroscopy. We focus our analysis on the description of the magnitude of the ground state charge transfer and on the details of the formed hybrid orbitals. Further, we show that for weakly bound donor / acceptor systems the FLO-SIC approach delivers a more realistic description of the electronic structure compared to standard DFT calculations.

This work has been supported by the Deutsche Forschungsgemeinschaft within the Research Unit FOR 1154 and ONR VSP N62909-16-1-2050.

Keywords: Density Functional Theory, Charge transfer, Electronic Structure, Self-interaction correction

A charge-charge-interacting monolayer under transverse bias: Order and current in

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We investigate a theoretical model for a monolayer of molecules or quantum dots sandwiched between two electrodes. Beside the equilibrium case, we also study the non-equilibrium setting given by a voltage-drop between the two electrodes.

In the case of weak tunneling between the monolayer and the electrodes a rate-equation approach is suitable. Solving the rate equation by a mean-field approximation as well as classical Monte Carlo simulations, we analyze the charge ordering and the perpendicular current for a square lattice with nearest-neighbor Coulomb repulsion.

We perform a comprehensive study of all phases at zero temperature with respect to all relevant model parameters, i.e. the bias voltage, the on-site energy and the degeneracy of the occupied single-site state.

One of the most remarkable findings is the prediction of a conducting charge-density-wave phase. This phase only appears for non-zero bias and a non-unity degeneracy of the occupied single-site state. The latter being a model for, e.g., the degeneracy of the electronic spin degree of freedom in the absence of a magnetic field.

Further we study the universality classes of the phase transitions towards the charge-ordered states. While all equilibrium transitions belong to the two-dimensional Ising universality class, this also holds for all non-equilibrium transitions at $T>0$ but not for all at $T=0$. Notable the zero-temperature bias-driven case exhibits an absorbing-to-active phase transition in the $\mathbb{Z}_2$-symmetric directed percolation (DP2) class.

Keywords:
Self-assembled films; Quantum dots; Sequential tunneling; Non-equilibrium thermodynamics

ALKALINE METAL DOPING OF ULTRATHIN FILMS OF METAL PHTHALOCYANINE

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It has been reported that doping of organic thin films by alkaline metals can considerably increase their electrical conductivity [1-2]. Especially for metal phthalocyanines site and orbital selective charge transfer and even spin manipulation by electron donating alkaline atoms has been demonstrated [3]. Understanding of the physical mechanisms behind these doping phenomena is prerequisite for application, especially in developing new effective materials for nano-devices like insulator-metal-insulator transistor [4], light emitting devices [5], photovoltaic cells [6], and so on.

Here the doping of a fluorinated cobalt phthalocyanine (F_{16}CoPc) monolayer surface by dilithium phthalocyanine (Li_2Pc) and Potassium (K) will be investigated by means of scanning tunneling microscopy and spectroscopy (STM/STS) in ultra-high vacuum. F_{16}CoPc is grown by organic molecular beam deposition (OMBD) on Au(111) and HOPG(0001) surfaces to prepare a crystalline ordered thin film. After that the small amount of Li_2Pc or Potassium has been co-deposited at the F_{16}CoPc to increase its conductivity. STM images and STS results collected at low temperatures reveal the charge transfer from F_{16}CoPc. In addition manipulating of doped molecules by applying voltage pulses to the STM tip will be demonstrated also.

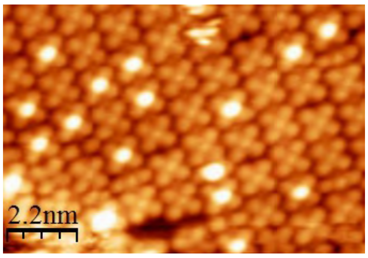

Fig. 1. STM image of F_{16}CoPc and Li_2Pc on Au(111)

Keywords: doped metal-phthalocyanine; F_{16}CoPc; Li_2Pc

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STM/STS INVESTIGATION OF PARAMAGNETIC MOLECULES

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The development of molecular nanostructures which contain magnetically bistable transition metal complexes arranged on planar surfaces is an active route towards materials with controllable magnetic or spintronic properties, leading to potential applications on information storage at the molecular level and molecular spintronics.

We study the molecular anchoring and electronic properties of different molecular nanostructures on metal surfaces by STM/STS. On type of structures are macrocyclic complexes fixed on gold surfaces [1]. Exchange-coupled macrocyclic complexes $[Ni_2L(Hmba)]^+$ were deposited ex-situ via 4-mer*cap*tobenzoate ligands on the surface of a Au(111) single crystal from solution in dichloromethane. The combined results from STM and XPS show the formation of large monolayers anchored via Au-S *bon*ds with a height of about 1.5 nm. Two apparent granular structures are visible: one related to the dinickel molecular complexes (cationic structures) and a second one related to the counter ions ClO_4^- which stabilize the monolayer. No type of short and long range order is observed. STM tip-interaction with the monolayer reveals higher degradation after eight hours of measurement. Spectroscopy measurements suggest a gap of about 2.5 eV between HOMO and LUMO of the cationic structures and smaller gap in the areas related to the anionic structures.

The other class of nanostructures is formed by endohedral metallofullerenes. Here, the monolayer formation depends strongly on the chosen metal substrate. In particular, if deposited on a W(110) surface the monolayer formation is inhibited by the strong immobility of the individual metallofullerenes. On the other hand, the Au(111) surface provides sufficient mobility to allow the formation of closed monolayers.

Paramagnetic Complexes: Self Assembled Monolayers; Endohedral Metallofullerenes; Scanning Tunneling Microscopy

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THE INFLUENCE OF CHLORINATION ON THE STRUCTURE AND VIBRATIONAL SPECTRA OF METALLOPHTHALOCYANINES

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Metallophthalocyanines (MePcs) are p-type organic semiconductors which possess attractive optical and electrical properties. Due to the low cost of their production and high thermal and chemical stability, MePcs as well as their junctions with other organic and inorganic semiconductors or metals, could be utilized for light-emitting diodes, photovoltaic cells, organic field effect transistors, sensors, and numerous other applications [1]. While pristine MePcs exhibit p-type behaviour due to the doping with electron accepting molecules, thin films of *e.g.* $ZnPcF_{16}$, were shown to exhibit n-type behavior [2]. The peripheral substitution of the conjugated macrocycle of MePcs by electron-withdrawing or electron-donating groups lowers the HOMO and LUMO levels (with respect the vacuum level), being a facile way to vary charge injection barrier, sensitivity and selectivity toward the different analytes, or other properties of the functional elements based on $MePcF_x$ or $MePcCl_x$ (x = 4, 8, 16).

Since the vibrational spectroscopy techniques (IR and Raman) are sensitive to the smallest changes of the structure and environment at the molecular level, they are particularly useful for the study of relatively weak binding interactions between MePcs and ligands or chemical analytes [3]. At the same time, although the vibrational spectra of H_2Pc and a series of MePcs (CuPc, ZnPc, FePc, CoPc, NiPc, etc.) have been well studied [3,4], much less reports can be found about vibrational structure spectra of their fluorinated and no studies of chlorinated counterparts.

In this work, based on the own experimental data and DFT calculations, we performed a detailed assignment of the vibrational bands in the Raman and FTIR spectra of a series of $MePcCl_8$-type MePcs (Me = Mn, Fe, Co, Ni, Cu). Further we discuss particular effects of the chlorination on the electronic structure of the molecules, as can be concluded from the behaviour of spectral features in the resonant Raman scattering experiments. Furthermore, the ordering of the $MePcCl_8$ molecules in thin films compared to that of their MePc counterparts will be reported

Keywords: Metallophthalocyanines; Raman spectroscopy; FTIR.

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Photoelectron spectroscopy studies of Phthalocyanine interfaces

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Transition-Metal-Phthalocyanines (TM-Pc) have attracted high interest in view of their potential for organic electronic applications. Interfaces are a central part of any device and the understanding of the electronic parameters at interfaces is essential for the understanding of the interfaces' behavior. Using photoelectron spectroscopy we have studied a number of interfaces of various phthalocyanines to partners such as simple metals, other TM-Pc and hydrocarbon based organic semiconductors. We summarize characteristic and intriguing results of these studies, which range from the formation of interface dipoles to the observation of a conducting (two-dimensional) layer induced by charge transfer across the interface.

This work has been supported by the Deutsche Forschungsgemeinschaft within the Research Unit FOR 1154.

Keywords: Transition Metal Phthalocyanine, Interfaces, Photoelectron Spectroscopy

Charge Transfer Channels Between Metal Phthaloycanines and Ferromagnetic Substrates

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The molecular orientation and the electronic structure of the metal phthalocyanines of FePc and CoPc on cobalt and nickel substrates were studied by near edge X-ray absorption fine structure (NEXAFS) spectroscopy. The results show thickness dependent orientation of these molecules on metal substrates, mainly influenced by the molecule-substrate interaction up to about 1 nm and by molecule-molecule interaction at higher film thicknesses. The suppression of the π-orbital features in the C 1s and N 1s NEXAFS spectra of FePc/Co and CoPc/Ni at the initial deposition stage indicates a charge transfer from the substrate to the pyrrole ring in the molecule. For CoPc/Co, however, C and N are far less involved in the charge transfer while the Co*3d* orbital accepts charge from the substrate which leads to the formation of an interfacial state at the Fermi level. Thus, both the center atom and the substrates play an important role in mediating the charge transfer at the interfaces.

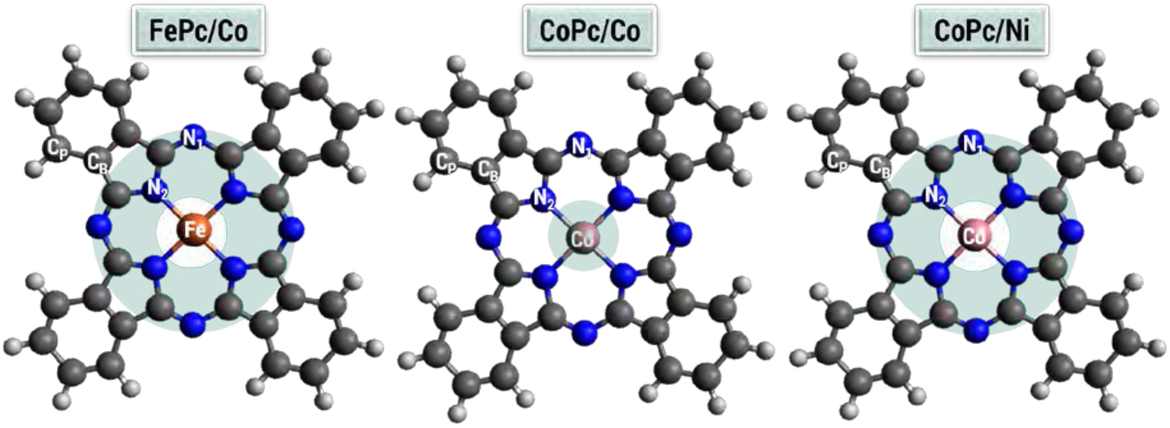

Fig. 1 Schematic diagram of different charge transfer channels for FePc/Co, CoPc/Co and CoPc/Ni. The shaded regions represent charge transfer channels at the interfaces.

Keywords: phthaloycanines, interfaces, charge transfer, molecular orientation

$La_{1-x}Sr_xMnO_3$ THIN FILMS ON SILICON PREPARED BY SPIN COATING: EFFECT OF THE STOICHIOMETRY ON THE MAGNETIC PROPERTIES

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$La_{1-x}Sr_xMnO_3$ (LSMO) is a promising electrode material for spintronic devices. The electrodes are typically deposited by pulsed laser deposition (PLD) on single crystal substrates with similar lattice constants, e.g. $SrTiO_3$ (STO) [1] to obtain single crystal layers. Especially the composition $x = 0.33$ is highly investigated because of the very high characteristic spin polarization. Alternatively, LSMO films are often deposited by magnetron sputtering, whereby we recently observed that the sputtering process usually yields a difference in stoichiometry between target and film. In this study we propose a more reliable deposition route for the fabrication of LSMO films from aqueous solutions by spin coating. This deposition method allows for easy tuning the stoichiometry. The composition of the films deposited onto (100) oriented silicon substrates covered with native oxide was set to be $x = 0.05$, 0.09, 0.19, 0.21, 0.28, 0.37, 0.44, and 0.74. After the spin coating the samples were annealed in ambient atmosphere for 1 hour at temperatures of 750 °C and 775 °C. The stoichiometry was verified by X-ray photoelectron spectroscopy (XPS) considering reflective electron energy loss spectroscopy (REELS) data for the evaluation. The Curie temperature, remanence and the coercive field of the layers were characterised by superconducting quantum interference device (SQUID) magnetometry. The results obtained show that in the range from $x = 0.15$ to $x = 0.40$ the Curie temperature is well above room temperature with a room temperature remanence of up to 60 %. These properties make the films suitable for applications in spintronic devices.

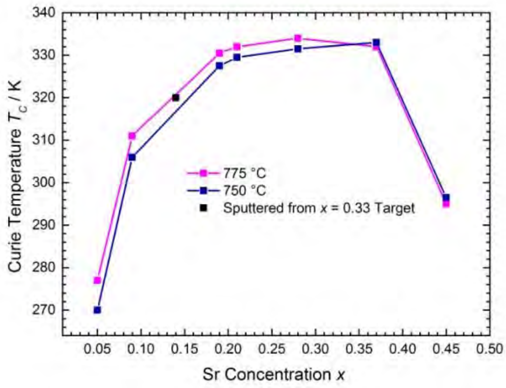

Fig. 1. Curie temperature over Sr concentration for films annealed at different temperatures

Keywords: LSMO, XPS, REELS, SQUID, Spin coating

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TIP-ENHANCED RAMAN SPECTROSCOPY: A METHOD TO OVERCOME DIFRACTION LIMIT

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The way to reach such nanoscale spatial resolution is possible only with a couple of advanced analytical techniques, particularly tip-enhanced Raman spectroscopy (TERS) offers many advantages. A scanning probe microscope (SPM) is required to couple to the Raman spectrometer so that a metallic tip of the SPM acts as the antenna to collect and amplify the signal from beneath the tip apex. Even thought it was already demonstrated that TERS can achieve sub-molecular resolution [1], practically, most experiments cannot be performed in high-vacuum and are non-conductive. In this light, the atomic force microscopy (AFM) feedback loop offers the most versatility.

In this contribution, we present AFM-TERS in ambient conditions with spatial resolution up to 5 nm. Here, to demonstrate the spatial resolution and the chemical analysis a sample carbon nanotubes on a gold substrate was employed.

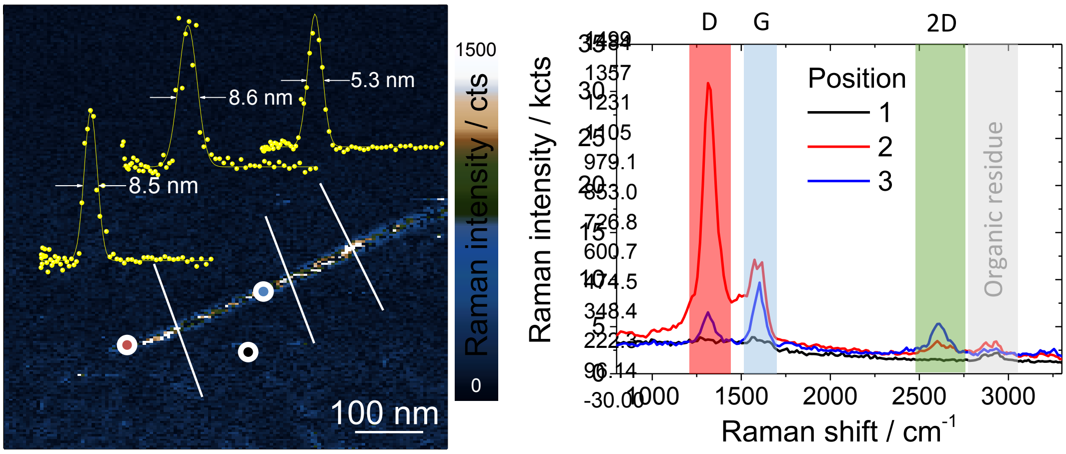

Fig. 1. Tip-enhanced Raman spectroscopy hyper-mapping. At each of the pixels was taken a Raman spectrum. The points are spaced 5 nm from each other. The spatial resolution is demonstrated by scanning over an intensity profile of the G band of carbon nanotubes.

Keywords: Raman spectroscopy, atomic force microscopy, carbon nanotubes, tip-enhanced Raman spectroscopy

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PHOTOSENSITIVE HYBRID TRENCH DEVICES BASED ON GOLD NANOPARTICLES INCORPORATED IN TIPS-PENTACENE MATRIX

S. Banerjee[a,b], **D. Bülz**[a], **D. Reuter**[b,c], **A. Raevskaya**[d], **V. Dzhagan**[a], **K. Hiller**[b], **D.R.T. Zahn**[a] **and G. Salvan**[a]

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Hybrid electronics offers opportunities to fabricate devices with enhanced performances combining the advantages of both organic and inorganic materials [1]. On the other hand in the last few decades, extensive studies have been carried out on preparation, characterization and application of metal nanoparticles [2] as the optical properties of such structures greatly differ from that of the bulk materials.

Here we demonstrate the light sensing properties of solution processed TIPS-pentacene based devices with trench isolated gold electrodes. Standard silicon processing technologies have been used to fabricate the trench devices. UV lithography is used to pattern sub-micron trenches which are in the next step partially filled with a layer of silicon oxide, which helps to achieve lower channel dimensions of the devices. Finally, a layer of Au is deposited to form the electrodes of the lateral devices. Such fabricated structures offer the advantage of accessing the active material of the devices from top, which is suitable for various sensor applications. TIPS-pentacene solution is then drop-coated on the devices, with or without gold nanoparticles incorporated in the TIPS-pentacene matrix. Device performances have been studied for different gold nanoparticle size and concentration of the gold nanoparticle dispersion in the TIPS-pentacene matrix. Three different laser lines (325 nm, 514.7 nm and 632.8 nm) have been used to investigate the light sensing properties of the fabricated devices in different wavelength regime.

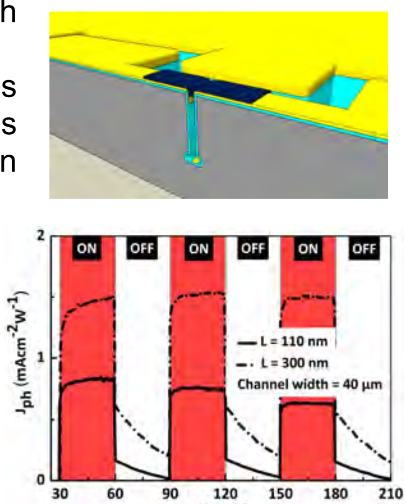

Fig. 1 Schematic diagram of the fabricated device(top). Photoconductive response of the device under 632.8 nm laser illumination

The obtained results suggest that this fabrication route for lateral devices can indeed be considered to be used for hybrid photodetectors.

Keywords: Hybrid device, Light sensing, Gold nanoparticles in TIPS-pentacene matrix

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INFLUENCE OF TEMPERATURE AND ILLUMINATION ON THE ELECTRICAL PROPERTIES OF LATERAL ORGANIC DEVICES

Daniel Bülz[a], **Sreetama Banerjee**[a], **Danny Reuter**[b], **Georgeta Salvan**[a] and **Dietrich R. T. Zahn**[a]

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In recent years electronic devices advanced rapidly and the need for new classes of materials has grown. In particular, organic semiconductors have come to great attention due to their tuneable properties regarding electronic band structure. They are also suitable for flexible electronics, which all together makes them promising candidates for curved or even flexible screens and photovoltaic devices.

In order to determine electrical properties of organic semiconductor films at nanoscale, a trench technique was developed to build lateral organic electronic devices with contact spacing below 100 nm. The device geometry yields in high electric field densities (1-2 orders of magnitude larger than the typical lateral devices with electrode spacing in the micrometer range), but grants direct access to the active channel.

Results of electrical characterization on this trench devices with 6,13-bis(triisopropylsilylethynyl)-pentacene (TIPS-pentacene) as active material will be shown as a function of temperature in the range from 150 K to 300 K. To explain the device performance, simulations for different geometries were performed with COMSOL Multiphysics®. Furthermore, experiments under laser illumination at a wavelength of 405 nm were carried out, to investigate the photoactivation of charge carriers in the electrically active channel. Our results show that the dominant charge transport mechanism in the devices is space charge limited current. Illumination of the active area with photons having energy above the HOMO-LUMO gap of the TIPS-pentacene reduces the effect of space charge limited charge transport mechanism.

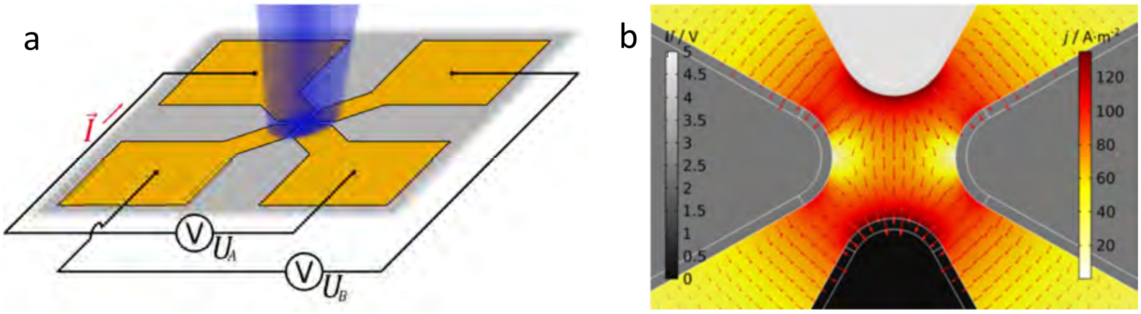

Fig. 1a) Shows a sketch of the trench structures with the measurement parameters and illumination geometry. 1b) Shows a current density map in the channel region simulated with COMSOL Multiphysics®.

Keywords: Organic Electronics; Temperature Dependence; Illumination; COMSOL Simulation

Templating Effects in Molecular Thin Films

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Controlling the molecular orientation in thin films is one of the main prerequisites in the rapidly growing fields of organic electronics and spintronics. Most organic molecules show a weak coupling to semiconducting or insulating surfaces which leads to disordered films. Phthaloycanines (Pcs) represent an outstanding class of molecules which physical and magnetic properties can be easily tuned. In addition they provide high thermal stability allowing the molecules to be sublimed in ultra-high vacuum (UHV) conditions [1]. It was previously shown that these molecules align parallel to the substrate surface when depositing a thin layer of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) beforehand [2]. This effect can further enhance optoelectronic [3] and magnetic properties [4]. In the case of cobalt phthalocyaine (CoPc) the ordering of the molecules in templated thin films can lead to magnetic coupling strengths (J/k_B = 80 K) that are larger than the thermal energy at the boiling point of liquid nitrogen [5]. Furthermore other molecules like tetracyanoquinodimethane (TCNQ) also exhibit templating effects originating from an additional PTCDA layer, although the driving forces are based on electrostatic and H-bonds, i.e. different to the π-π interactions inducing templating in Pcs [6].

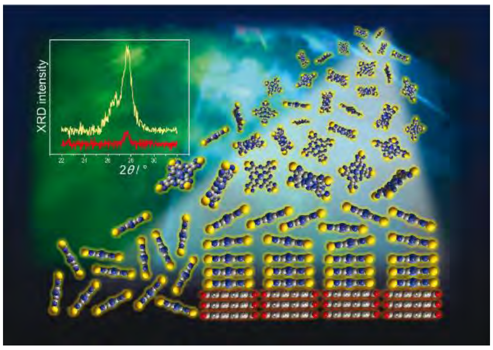

Fig. 1. CoTTDPz thin films on bare substrates and PTCDA.

In this work we present the templating effect of PTCDA on the growth of cobalt tetrakis(thiadiazole)porphyrazine (CoTTDPz) thin films [7]. While X-ray diffraction and optical absorption show that CoTTDPz films on bare substrates are amorphous they are highly ordered when the molecules are deposited on PTCDA, inducing the appearance of a strong antiferromagnetic coupling.

Keywords: Molecular orientation; Templating effects; PTCDA

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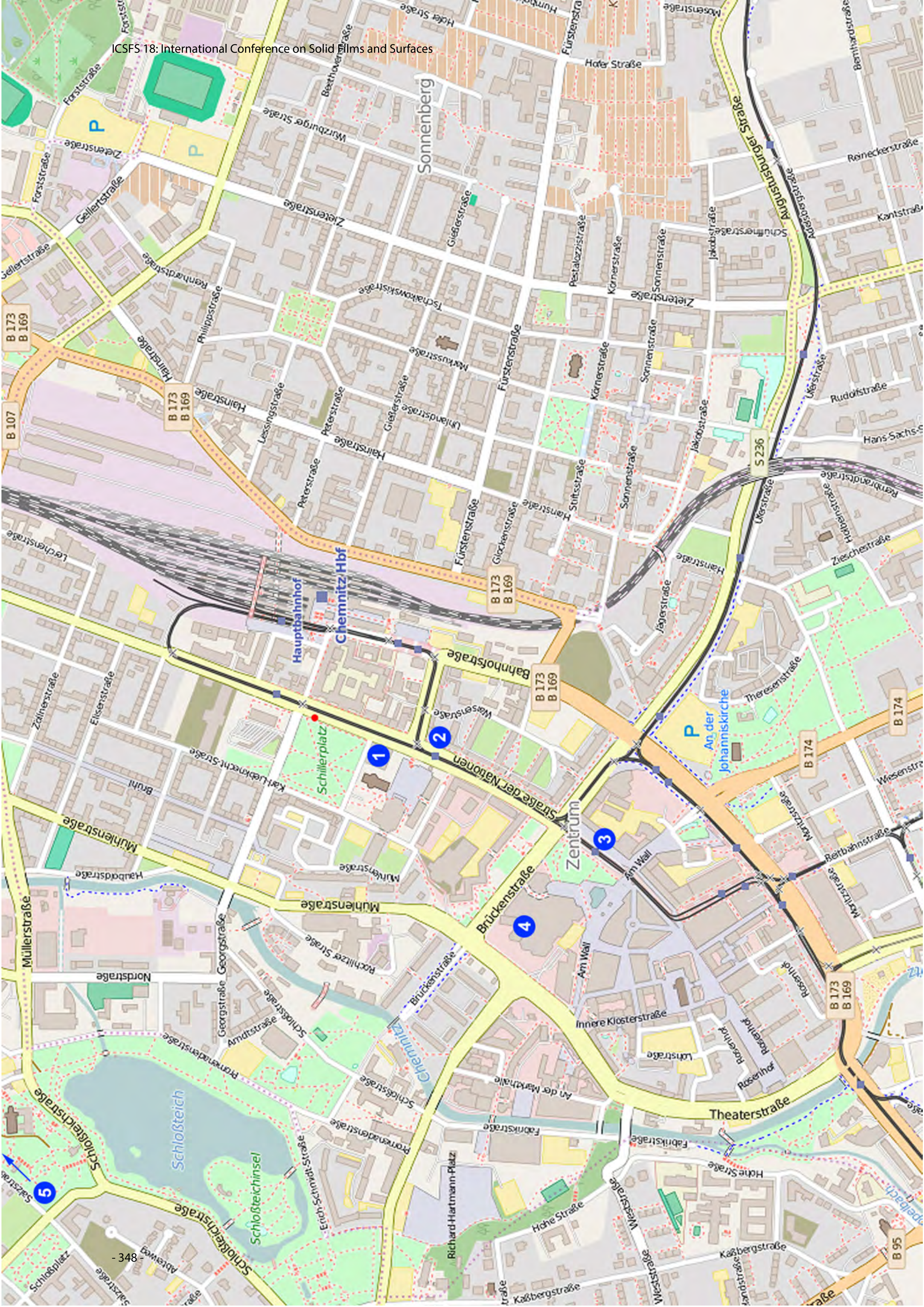
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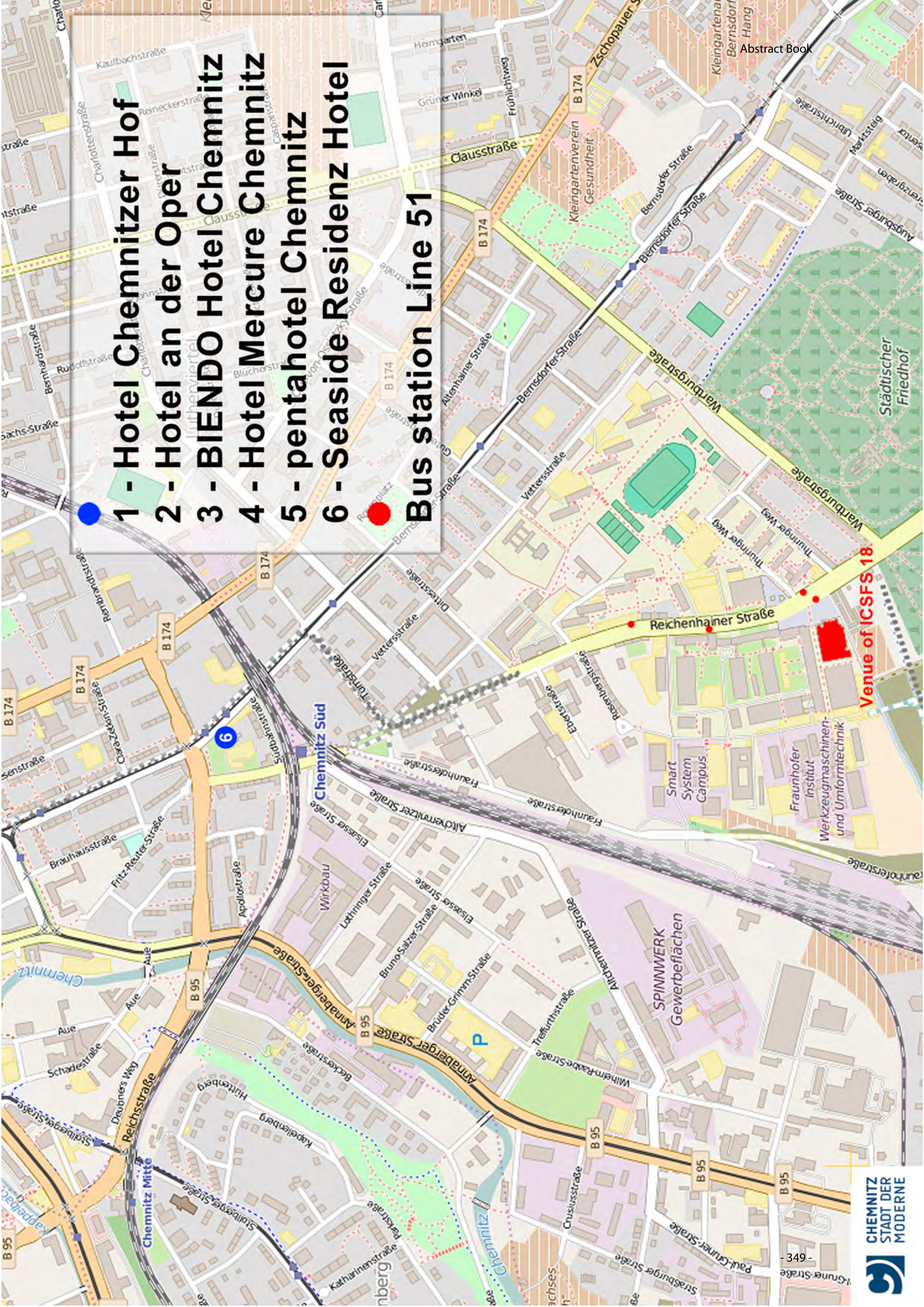
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