ICFSI
2017

Scientific Program

July 2 – 7, 2017

Hannover Congress Centrum

www.icfsi-16.org
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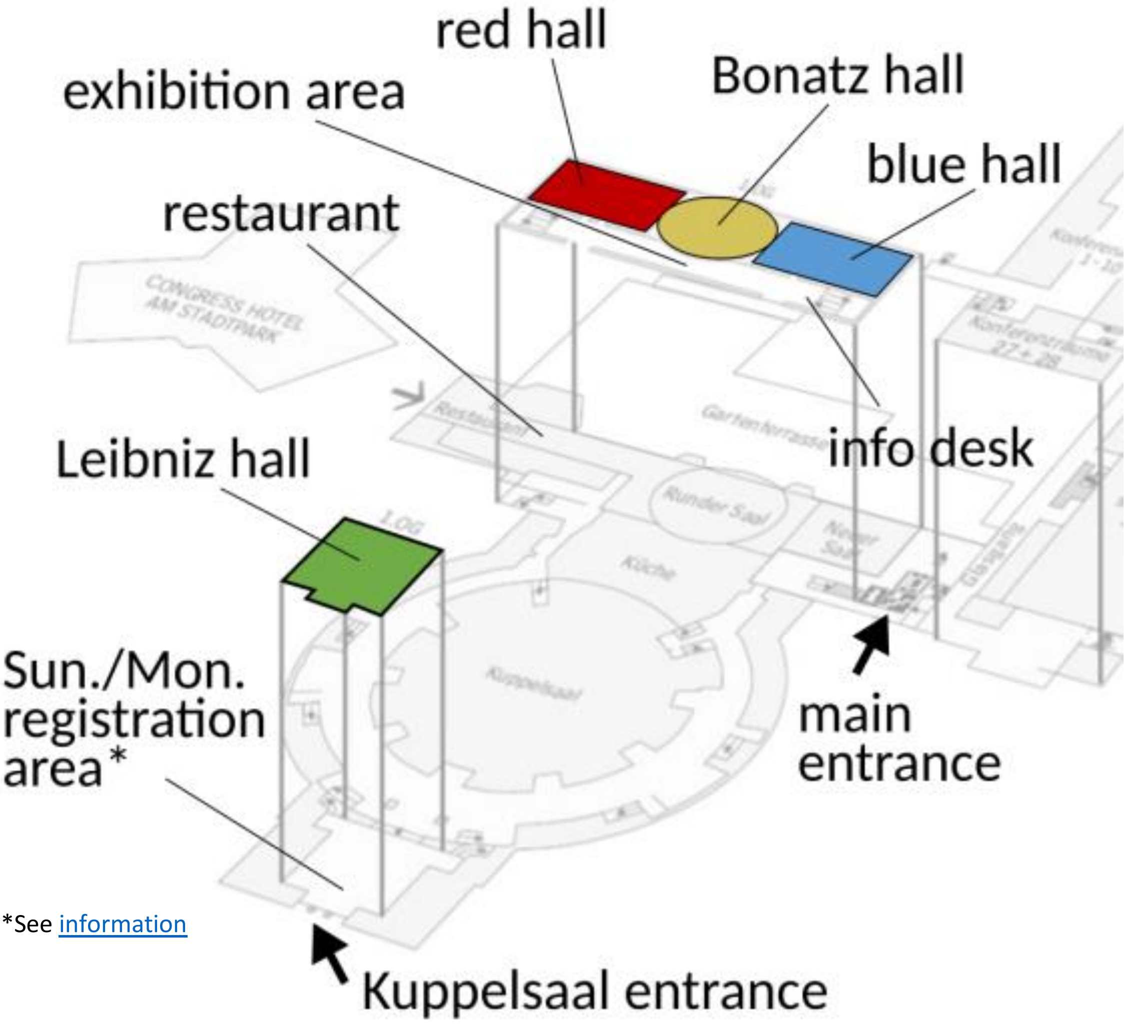
HCC site map and important information



*See information

Wifi

Network: Leibniz-Universität
Password: ICFSI2017

Venue

Hannover Congress Centrum (HCC)
Theodor-Heuss-Platz 1-3
30175 Hannover

Emergency Number

Ms. Heike Kahrs (Secretary)
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Monday Tuesday Wednesday Thursday Friday Posters Author Index

Welcome to the 16th International Conference on the Formation of Semiconductor Interfaces (ICFSI-16) in Hannover!

Hannover is located close to the center of Germany. It is a lively modern city that combines modern lifestyle ("greenest city of Germany") with tradition at its historic sites. Being the economic heart of the state of Lower Saxony, it is also an important center of music, art, and science. The recent celebration of the Leibniz year in 2016, memorizing the activities and achievements of the great mathematician, engineer, and philosopher Gottfried Wilhelm Leibniz reflects this symbiosis best.

This 16th conference of the ICFSI series, started in 1985 by G. Le Lay, has the intention, as all previous meetings, to give a broadband overview over the latest developments of modern phenomena at surfaces, interfaces, and nanostructures based on semiconductors or insulators ranging from the characterization at the atomic scale to prospects of electronic, spintronic, photonic and photovoltaic applications. The aim for this conference is to bring together leading experts from various fields and disciplines in order to stimulate the exchange of knowledge and promote the capabilities of this interdisciplinary research topic.

We as the organizers hope that this meeting will again be a lively and fruitful forum for scientific exchange and for discussions in the interdisciplinary fields of low-dimensional physics, nanoscience, interfaces, surfaces and nanostructures. We hope that you will have a pleasant stay at this conference, in Hannover and in Germany.

The local organizing committee

Monday Tuesday Wednesday Thursday Friday Posters Author Index

Further information

Directions to the venue

The following sites will give you information about how to find your way to the Congress Centrum and around Hannover: www.gvh.de, www.efa.de, and www.bahn.de.

Public transport from Hannover main station (Taxi costs est. 10€): Either take the bus line 128 or 134 in direction Peiner Straße or after a short walk to the station Kröpcke, the subway line 11 to the Zoo and Congress Centrum. The stop is directly at the Congress Centrum.

Registration desks

On Sunday and Monday, the registration desks are located at the Kuppelsaal entrance. On all other days, the registration is possible in front of the Leibniz hall in the early morning and at an additional information desk in front of the red and blue hall after the plenary talks. On Sunday, the registration opens at 17:00, on Monday at 7:45 and on all other days at 8:30.

Certificate of attendance

You receive the certificate of attendance during the registration together with all informational material.

Welcome reception

The welcome reception takes place in the HCC restaurant.

Coffee breaks

During the coffee breaks, coffee and other hot beverages as well as cookies, sweets, and fruits are served in the exhibtion area.

Lunch breaks

A buffet style lunch is served in the exhibition area at no extra cost during lunch breaks in the exhibition area. See program for lunch break times.

Conference outing

The busses depart in front of the main entrance on Wednesday at 14:00.

Conference dinner

The conference dinner takes place in the HCC restaurant. You have to be registered to participate. If you booked a ticket during online registration, you receive a dinner ticket together with your conference badge. It is still possible to buy a ticket at the registration desk during the conference until Tuesday.

Internet connection

Access to the WIFI "Leibniz-Universität" is granted with the password "ICFSI2017".

Poster session

The presenters are asked to put up their posters on Monday. A focused poster session takes place on Thursday from 11:05 in the Bonatz hall.

Poster award

The best three posters are awarded a poster prize that is announced during the conference dinner.

Book of abstracts

Abstracts of the contributions can be found on the flash drive you received during registration or on www.icfsi-16.org.

Exhibition

An exhibition takes place in the Bonatz hall and a designated area in front of the blue and red hall from Tuesday to Thursday.

History

The ICFSI series was initiated in 1985 in Marseille, France by an initiative of Prof. Le Lay who was the chairman of ICFSI-1. The ICFSI conferences following in series took place in:

- Takarazuka, Japan in 1988; chaired by Prof. A. Hiraki
- Rome, Italy in 1991; chaired by Dr. P. Perfetti
- Jülich, Germany in 1993; co-chaired by Prof. H. Lüth and W. Mönch
- Princeton, NJ, USA in 1995; co-chaired by Prof. A. Kahn and Dr. R. Ludeke
- Cardiff, Wales, UK in 1997; chaired by Prof. R. Williams
- Göteborg, Sweden in 1999; chaired by Prof. P. O. Nilsson
- Sapporo, Japan in 2001; chaired by Prof. H. Hasegawa
- Madrid, Spain in 2003; chaired by Prof. F. Flores
- Aix en Provence, France in 2005; co-chaired by Prof. P. Soukiassian and G. Le Lay
- Manaus, Brazil in 2007; co-chaired by Prof. E. F. da Silva Jr. and A. Ferreira da Silva
- Weimar, Germany in 2009; co-chaired by Prof D. R. T. Zahn and F. Bechstedt
- Prague, Czech Republic in 2011; co-chaired by Prof. P. Jelinek and V. Chab
- Gyeongju, South Korea in 2013; co-chaired by Prof. H. W. Yeom and C. Y. Park
- Hiroshima, Japan in 2015; chaired by Prof. A. Kimura

Scope

ICFSI-16 will primarily focus on phenomena at surfaces, interfaces, and nanostructures that are of strong current interest, based on semiconductor or insulator surfaces and interfaces, ranging from characterization at the atomic scale to prospects of applications.

The following aspects will be covered by the conference:

- Surfaces and interfaces of topological materials
- Spins at semiconductor surfaces and interfaces
- Quasi-one-dimensional structures
- Metal-semiconductor and insulator-semiconductor interfaces
- Graphene and its interfaces
- Interfaces with oxides
- Organic semiconductor interfaces
- Heterojunctions
- Functionalization and chemical aspects of surfaces and interfaces
- Oxides, nitrides, and high-k dielectrics
- Advanced experimental techniques for surface and interface characterization
- State-of-the-art theoretical approaches
- Frontier applications of semiconductors, surfaces, and interfaces
- Nanoelectronics, molecular electronics, nanophotonics, and spintronics
- Emergent two-dimensional materials, e.g. TMDCs, Silicene, etc.
- And others

Steering committee

- A. A. Saranin (Institute of Automation and Control Processes, Wladiwostok, Russia)
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- D. R. T. Zahn (Chemnitz University of Technology, Germany)
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- Prof. Dr. Herbert Pfnür
- Prof. Dr. Christoph Tegenkamp
- Prof. Dr. Eric Jeckelmann
- Timo Lichtenstein
- Frederik Edler
- Heike Kahrs

Course of events

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Sunday, July 2

17:00	Opening of registration
18:00	Welcome reception

Monday, July 3

8:45 – 9:00	Opening ceremony with **Prof. Dr. Volker Epping** President of the Leibniz University of Hannover
9:00 – 9:45	Plenary talk – Leibniz hall **Taro Hitosugi (Tokyo Institute of Technology, Japan)** *Atomistic understandings of perovskite oxide surfaces using scanning tunneling microscopy*
9:50 – 12:50	Session: “2D superconductivity” – blue hall
9:50 – 13:00	Session: “Applied surface science I” – red hall
13:00 – 14:30	Lunch break
14:30 – 18:00	Session: “Semiconductors and semiconductor interfaces” – blue hall
14:30 – 17:45	Session: “Functionalization of semiconductor interfaces I” – red hall

Tuesday, July 4

9:00 – 9:45	Plenary talk – Leibniz hall **Philip Hofmann (Aarhus University, Denmark)** *Electronic structure of novel two-dimensional materials*
9:50 – 13:20	Focused session: “Dynamics at surfaces” – Leibniz hall
13:00 – 14:30	Lunch break
14:30 – 18:20	Session: “Interfaces of layered materials” – blue hall
14:30 – 17:20	Session: “Functionalization of semiconductor interfaces II” – red hall

Wednesday, July 5

9:00 – 9:45	Plenary talk – Leibniz hall **Dimitrie Culcer (University New South Wales, Australia)** *Quantum computing with rough multi-valley Si systems:* *electrically-driven spin and valley resonances and overcoming roughness*
9:50 – 13:00	Session: “Organic molecules, layers, and electronics I” – blue hall
9:50 – 12:20	Session: “Spins at surfaces and interfaces I” – red hall
9:50 – 13:00	Session: “Graphene I” – Leibniz hall
13:00 – 14:00	Lunch break
14:00	Conference outings – departure in front of the main entrance

Thursday, July 6

9:00 – 9:45	Plenary talk – Leibniz hall **Han Woong Yeom (Pohang, Korea)** *Chiral solitons in atomic wires:* *towards multi-digit topological computation*
9:50 – 11:05	Session: “Nanowires and atomic wires I” – blue hall
9:50 – 11:05	Session: “Spins at surfaces and interfaces II” – red hall
9:50 – 11:25	Session: “Graphene II” – Leibniz hall
11:00 – 13:00	Poster session – Bonatz hall
13:00 – 14:30	Lunch break
14:30 – 16:10	Session: “Nanowires and atomic wires II” – blue hall
14:30 – 17:20	Session: “Applied surface science II” – red hall
16:25 – 17:35	Session: “Spins at surfaces and interfaces III” – blue hall
19:00	Conference dinner – HCC restaurant

Friday, July 7

9:30 – 11:40	Session: “Organic molecules, layers, and electronics II” – blue hall
9:30 – 12:05	Session: “Topological insulators” – red hall
12:15	Closing remarks and end of conference – red hall

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Detailed program

Monday, July 3

8:45	Opening ceremony	with Prof. Dr. Volker Epping President of the Leibniz University of Hannover
9:00	**Plenary talk: Taro Hitosugi (Tokyo Institute of Technology, Japan)**	Atomistic understandings of perovskite oxide surfaces using scanning tunneling microscopy

Session: "2D superconductivity" (9:50 – 12:50) – blue hall

9:50	**Invited talk: Dimitri Roditchev (ESPCI and INSP Paris, France)**	Coherent quantum phenomena in superconducting atomic monolayers Pb/Si(111): A STM study
10:25	**Invited talk: Felix von Oppen (Freie Universität Berlin, Germany)**	From Majorana bound states to topological quantum computation
11:00	*Coffee break*	
11:25	**Invited talk: Shuji Hasegawa (The University of Tokyo, Bunkyō-ku, Japan)**	Atomic-Layer Superconductors
12:00	**Invited talk: Jin-feng Jia (Shanghai Jiao Tong University, China)**	Majorana Fermion in the Vortex of Topological Superconductors by proximity effects
12:35	Takashi Uchihashi (National Institute for Materials Science, Japan)	Giant In-plane Critical Fields of Superconducting Atomic Layers on Silicon

Session: "Applied surface science I" (9:50 – 13:00) – red hall

9:50	**Invited talk: Stephan Wippermann (MPI für Eisenforschung, Germany)**	Characterizing buried nano-interfaces in nanocrystal solids at the atomistic level: a coupled theoretical-experimental approach
10:25	Simon Charbonnier (Institut de Physique de Rennes, France)	GaP/Si(001) polar-on-nonpolar epitaxial growth revisited by scanning tunneling microscopy
10:45	Martin Franz (Technische Universität Berlin, Germany)	Towards atomic-scale switches based on self-assembled magic clusters
11:05	*Coffee break*	
11:25	**Invited talk: Emmanuelle Deleporte (Aimé Cotton Laboratory, France)**	Excitonic emission of hybrid lead iodide perovskite single crystals
12:00	Jonas Köhling (Jacobs University Bremen, Germany)	Effect of β-diketone passivation on solution processed zinc oxide nano-layers used in thin film transistors
12:20	Eugen Speiser (ISAS Berlin, Germany)	Resonant Raman scattering at surface vibrational modes of clean and O-terminated Cu(110)
12:40	Michael Meyer (SPECS Surface Nano Analysis, Germany)	New Instrumentation for spin-integrated and spin-resolved Momentum microscopy – METIS and KREIOS

Lunch break (13:00 – 14:30)

Session: "Semiconductors and semiconductor interfaces" (14:30 – 18:00) – blue hall

14:30	**Invited talk: Paul Koenraad (Eindhoven University, the Netherlands)**	Magnetic interactions in artificially created Mn assemblies in a GaAs (110) surface
15:05	Heiko Bremers (TU Braunschweig, Germany)	X-Ray reflectivity measurements of ultrathin layers in 2DEG AlGaN structures
15:25	Yasuo Cho (Tohoku University, Japan)	Local deep level transient spectroscopy for two-dimensional MOS interface characterization based on scanning nonlinear dielectric microscopy
15:45	Martin Wenderoth (Universität Göttingen, Germany)	Electronic properties of the Fe/GaAs(110) interface
16:05	*Coffee break*	
16:25	**Invited talk: Neil Curson (London Centre for Nanotech., UCL, Great Britain)**	Non-destructive imaging of atomically-thin nanostructures buried in silicon
17:00	Mario Dähne (TU Berlin, Germany)	Electronic structure of the non-polar GaN(10–10) surface
17:20	Uwe Rossow (TU Braunschweig, Germany)	Indium incorporation related surface processes during InGaN quantum well growth
17:40	Andrey Zotov (IAPU, Vladivostok, Russia)	Exotic 2D nanostructures of adsorbates on silicon

Session: "Functionalization of semiconductor interfaces I" (14:30 – 17:45) – red hall

14:30	**Invited talk: Marius Grundmann (University of Leipzig, Germany)**	Interfacing Bragg Mirrors with Tilted Uniaxial Media: Exceptional Points and Chiral States
15:05	Nicola Gaston (The University of Auckland, USA)	Engineering the surface states of ZnO and SnO2
15:25	Lukas Gierster (Fritz-Haber-Institut, Germany)	Ultrafast electron transfer across a ZnO-organic interface
15:45	Qiankun Wang (Humboldt University Berlin, Germany)	Photochromic phosphonic-acid diarylethene self-assembled monolayer switches on polar ZnO surfaces
16:05	Coffee break	
16:25	Gholamreza Nabiyouni (Arak University, Iran)	Kinetic roughening study in electrodeposited films
16:45	Hugo Dil (Ecole polytechnique, Lausanne, Switzerland)	Manipulation of 2D states on the surfaces of transition metal oxides
17:05	Que Huong Nguyen (Marshall University, USA)	Phonon Mediated Optical Stark Effect for Hybrid Heterostructures
17:25	Hoa Hong Nguyen (Seoul National University, Korea)	Magnetic Transition-Metal-doped ZrO2 Thin Films for Spintronic Applications

Tuesday, July 4

9:00	**Plenary talk: Philip Hofmann (Aarhus University, Denmark)**	Electronic structure of novel two-dimensional materials

Focused session: “Dynamics at surfaces” (9:50 – 13:20) – Leibniz hall

9:50	**Invited.talk: Michael Horn-von Hoegen (Universität Duisburg-Essen, Germany)**	1D Atomic Wires at Surfaces: Ultrafast non-Equilibrium Structural Dynamics in the Si(111)-In (8x2)<>(4x1) System at the Quantum Limit
10:25	**Invited talk: Ulrich Höfer (Philipps-Universität Marburg, Germany)**	Time-resolved spectroscopy of electron transfer processes at metal/organic interfaces
10:50	**Invited talk: Uwe Bovensiepen (Universität Duisburg-Essen, Germany)**	Excitations driven by femtosecond laser pulses in complex materials: Challenges and opportunities
11:15	**Invited talk: Martin Wolf (Fritz-Haber-Institut Berlin, Germany)**	Ultrafast Electronic Structure Changes during Photoinduced Phase Transitions: The Dynamics of the In/Si(111) (8x2) ↔ (4x1) Transition
11:40	*Coffee break*	
12:00	**Invited talk: Claus Ropers (Universität Göttingen, Germany)**	Ultrafast Low-Energy Electron Diffraction Enabled by Nanoscale Photoemitters
12:25	**Invited talk: Frank Meyer zu Heringdorf (Universität Duisburg-Essen, Germany)**	Ultrafast dynamics of surface plasmon polaritons
12:50	**Invited talk: Beatrice Andres (Freie Universität Berlin, Germany)**	Electron dynamics in the Rashba system BiTeI

Lunch break (13:15 – 14:30)

Session: “Interfaces of layered materials” (14:30 – 18:20) – blue hall

14:30	**Invited talk: David Bowler (Dep. of Physics & Astronomy, UCL, Great Britain)**	Defects, doping and the CDW in TiSe2
15:05	**Invited talk: Christoph Renner (University of Geneva, Switzerland)**	Thickness dependence of the charge density wave order parameter in thin exfoliated 1T-VSe2
15:40	Stefan Heun (NEST, Istituto Nanoscienze-CNR, Pisa, Italy)	Dephasing in Strongly Anisotropic Black Phosphorus
16:00	*Coffee break*	
16:15	**Invited talk: Harold J. W. Zandvliet (University of Twente, the Netherlands)**	Germanene: graphene's little sister
16:50	**Invited talk: Giancarlo Cicero (Politecnico di Torino, Italy)**	MoS2 enhanced T-phase stabilization and tunability through alloying and organic functionalization
17:25	**Invited talk: Ken Shih (University of Texas, Austin, USA)**	Probing atomic and electronic structures of 2D electronic materials and their heterostructures
18:00	Marcelo Marques (Instituto Tecnologico de Aeronautica, Brasil)	Interfaces between two atomically thin layers: structure and electronic properties

Session: "Functionalization of semiconductor interfaces II" (14:30 – 17:20) - red hall		
14:30	**Invited talk: Eric Mattson (University of Texas at Dallas, USA)**	Mechanistic Studies of Monolayer Doping of Semiconductor Surfaces for Ultra-shallow Junctions
15:05	Dietrich Zahn (Technical University of Chemnitz, Germany)	Au Nanoantenna Arrays for Surface-enhanced IR Absorption
15:25	Alexander Saranin (IAPU, Vladivostok, Russia)	Atomic structure and electronic properties of the 2D Tl-based compounds with √3×√3 periodicity on the Si(111) surface
15:45	*Coffee break*	
16:05	**Invited talk: Michael Flatté (University of Iowa, USA)**	Spin dynamics of individual magnetic impurities at the surface of a semiconductor
16:40	Steven Schofield (University College London, Great Britain)	Quantum states of atomic defect nanostructures in silicon
17:00	Taylor Stock (London Centre for Nanotech., UCL, Great Britain)	Si(001)-AsH3 : Arsine as Precursor to STM Patterned 2D Arsenic in Silicon

Wednesday, July 5

9:00	**Plenary talk: Dimitrie Culcer (University New South Wales, Australia)**	Quantum computing with rough multi-valley Si systems: electrically-driven spin and valley resonances and overcoming roughness

Session: "Organic molecules, layers, and electronics I" (9:50 – 13:00) – blue hall

9:50	**Invited talk: Guillaume Schull (CNRS - Strasbourg, France)**	STM-induced light emission: from molecular LED to subnanometric optical microscopy
10:25	**Invited talk: Frank Palmino (Institut FEMTO-ST, CNRS, France)**	Molecular self-assembled networks on boron doped silicon surface
11:00	*Coffee break*	
11:25	**Invited talk: Willi Auwärter (Technical University of Munich, Germany)**	Interfaces of functional molecules with graphene and h-BN
12:00	Kirill Bobrov (Inst. des Sciences Moléculaires d'Orsay, France)	Accommodation of the self-assembled perylene multilayer to Ag(110) surface morphology.
12:20	Giuseppe Foti (Inst. of Physics, Czech Academy of Science)	Current-induced heating of carbene-based molecular junctions controlled by the interface
12:40	Ziad Khattari (Hashemite University, Jordan)	Adsorption kinetics of low density lipoproteins with Langmuir monolayer

Session: "Spins at surfaces and interfaces I" (9:50 – 12:20) – red hall

9:50	**Invited talk: Jörg Schäfer (University of Würzburg, Germany)**	Realization of Bismuthene – A Novel Two-Dimensional Material as High-Temperature Quantum Spin Hall Candidate
10:25	**Invited talk: Markus Donath (Universität Münster, Germany)**	Spin-momentum-locked valleys in metal/semiconductor hybrid systems
11:00	*Coffee break*	
11:25	**Invited talk: Pedro Miguel Echenique (Donostia International Physics Center, Spain)**	Surface Attophysics
12:00	Hendrik Bentmann (Universität Würzburg, Germany)	Spin-texture inversion in the giant Rashba semiconductor BiTeI

Session: "Graphene I" (9:50 – 13:00) – Leibniz hall		
9:50	**Invited talk: Thomas Seyller (Technische Universität Chemnitz, Germany)**	Polarization Doping and Work Function of Epitaxial Graphene on Silicon Carbide
10:25	**Invited talk: Thomas Michely (Universität zu Köln, Germany)**	Graphene as a substrate: 2D layer van der Waals epitaxy and 1D nanowires
11:00	*Coffee break*	
11:25	**Invited talk: An Ping Li (Oak Ridge National Lab, USA)**	Spin-Polarized Four-Probe STM Study on Spin Transport of Topological Insulators
12:00	Benfdila Arezki (University M. MAMmeri Tizi-Ouzou, Algeria)	Investigation on Metal-Graphene-Semiconductor (MGS) Interfaces
12:20	Alexander Chaika (ISSP RAS, Chernogolovka, Russia)	Few-layer graphene with self-aligned nanodomain boundaries on SiC/Si(001): Atomic structure, transport and magnetic properties
12:40	Fumio Komori (University of Tokyo, Chiba, Japan)	Modulation of electron-phonon coupling in one-dimensionally nanorippled graphene on a macrofacet of 6H-SiC

Lunch break (13:00 – 14:00)

Conference Outing (from 14:00) – departure in front of the main entrance

Thursday, July 6

9:00	**Plenary talk: Han Woong Yeom (POSTECH, Pohang, Korea)**	Chiral solitons in atomic wires: towards multi-digit topological computation

Session: “Nanowires and atomic wires I” (9:50 – 11:05) – blue hall

9:50	**Invited talk: Philipp Ebert (Forschungszentrum Jülich, Germany)**	Band offsets and ordering in III-V nanowires determined by STM and STS
10:25	Stephan Appelfeller (Technische Universität Berlin, Germany)	Clarifying the electronic structure of rare earth silicide nanowires on Si(001)
10:45	Joachim Wollschläger (Universität Osnabrück, Germany)	Strain induced quasi-one dimensional structure of rare earth silicides on Si substrates

Session: “Spins at surfaces and interfaces II” (9:50 – 11:05) – red hall

9:50	**Invited talk: Koichiro Yaji (The University of Tokyo, Japan)**	Spin polarization of spin-orbit coupled states studied by laser-SARPES
10:25	Joerg Malindretos (Universität Göttingen, Germany)	Weak spin injection in epitaxial MnGa/GaN
10:45	Pascal Turban (Rennes 1 University , France)	Ballistic Emission Electron Microscopy investigation of the spin filtering effect in epitaxial Fe/Au/Fe/GaAs(001) spin valve

Session: “Graphene II” – Leibniz hall (9:50 – 11:25) – Leibniz hall

9:50	**Invited talk: Alexander Shikin (Saint Petersburg State University, Russia)**	Topological phase, spin-orbit and exchange coupling induced in graphene under contact with heavy and magnetic metals
10:25	Jean-Christophe Le Breton (Institut de Physique de Rennes, France)	Band Alignments in Fe/Graphene/Si(001) Junctions Studied by X-ray Photoemission Spectroscopy
10:45	Vyacheslav Silkin (Donostia Int. Physics Center, Spain)	Temperature versus doping effects on low-energy plasmons in graphene
11:05	Shiyong Wang (Empa, Materials Science and Tech., Switzerland)	Quantum Dots in Graphene Nanoribbons

Poster session (11:05 – 13:00) – Bonatz hall

Lunch break (13:00 – 14:30)

Session: “Nanowires and atomic wires II” (14:30 – 16:10) – blue hall

14:30	Martin Hohenadler (University of Würzburg, Germany)	Interplay of bond and site electron-phonon coupling in one dimension
14:50	Samad Razzaq (MPI für Eisenforschung, Germany)	Pinning of topological solitons at extrinsic defects in a quasi-one-dimensional charge density wave
15:10	Ryszard Zdyb (Maria Curie-Sklodowska University, Lublin, Poland)	One-dimensional metallic nanostructures on highly anisotropic silicon surfaces
15:30	Julian Plaickner (ISAS Berlin, Germany)	Functionalization of Si(553)-Au surface with hydrogen and small organic molecules
15:50	Timo Lichtenstein (Leibniz Universität Hannover, Germany)	What we can learn from plasmons in gold induced wires on Si(hhk)

“Spins at surfaces and interfaces III” (16:25 – 17:35) – blue hall

16:25	**Invited talk: Akio Kimura (Hiroshima University, Japan)**	Probing non-equilibrated Dirac fermions on surface of topological insulators
17:00	**Invited talk: Paolo Sessi (Universität Würzburg, Germany)**	Edge states at topological crystalline insulator surfaces: a new approach towards robust 1D modes

Session: “Applied surface science II” (14:30 – 17:20) – red hall

14:30	**Invited talk: Thomas Hannappel (TU Ilmenau, Germany)**	Scrutinizing the III-V-on-Si interface formation on the atomic scale in situ and by DFT
15:05	Juan Rubio-Zuazo (Instituto de Ciencia de Materiales de Madrid, Spain)	Determination of electronic and atomic properties of surface, bulk and buried interfaces: Simultaneous combination of hard X-ray photoelectron spectroscopy and X-ray diffraction
15:25	Thorsten Schultz (Humboldt-Universität zu Berlin, Germany)	Work function measurements of bilinear self-assembled monolayer arrays: The role of electrostatic potentials for Ultraviolet Photoelectron Spectroscopy
15:45	Miguel Manso Silvan (Universidad Autónoma de Madrid, Spain)	Porous silicon distributed Bragg reflector-Au nanocavity based dual sensing structures
16:05	*Coffee break*	
16:25	Mohammed Shabat (Islamic Oniversity of Gaza, Palestine)	Multi-layered waveguide silicon structure for solar cells models
16:45	**Invited talk: Pere Roca i Cabarrocas (Université Paris-Saclay, France)**	Low temperature plasma epitaxy of Silicon on III-V for tandem solar cells

Conference dinner (19:30) – HCC restaurant

Friday, July 7

Session: "Organic molecules, layers, and electronics II" (9:30 – 11:40) – blue hall

9:30	**Invited talk: Stefan Müllegger (Johannes Kepler University Linz, Austria)**	Radio-frequency scanning tunneling microscopy on molecular and atomic resonators
10:05	Daijiro Nozaki (University of Paderborn, Germany)	Molecular Orbital Rule for Quantum Interference in Weakly Coupled Dimers: Low-Energy Giant Conductivity Switching Induced by Orbital Level Crossing
10:25	Diana Slawig (Leibniz Universität Hannover, Germany)	Resonances in electron transport through single molecules of Ferrocene-dithiol
10:45	*Coffee break*	
11:05	**Invited talk: Richard Berndt (IEAP, CAU Kiel, Germany)**	A microscopic view of atomic and molecular contacts

Session: "Topological insulators" (9:30 – 12:05) – red hall

9:30	**Invited talk: Sergey Eremeev (ISPMS, Tomsk, Russia)**	Emergence of topologically non-trivial phases in systems consisting of the structure elements of layered giant-Rashba band insulators
10:05	Friedhelm Bechstedt (Friedrich-Schiller-Universität Jena, Germany)	Quantum spin Hall conductivity in 2D crystals
10:25	Chiara Bigi (Università degli Studi di Milano, Italy)	Spin-resolved and angular-resolved photo-emission spectroscopy experiments on in-situ transferred epitaxial Bi2Se3 thin films
10:45	*Coffee break*	
11:05	Felix Lüpke (Forschungszentrum Jülich, Germany)	Electrical resistance of individual defects at a topological insulator surface
11:25	Bert Voigtländer (Forschungszentrum Jülich, Germany)	Disentangling in situ top and bottom conductance of a topological insulator thin film

End of conference and closing remarks (12:15) – red hall

List of Posters

Poster A: "Adsorption on surfaces" – Bonatz hall		
A.1	John Adongo (Helmholtz-Zentrum Berlin, Germany)	Towards a Renewable Modified Surface for Rapid Sensing and Chelation of Heavy Metal ion Pollutants
A.2	Stefan Borgsdorf (Ruhr-Universität Bochum, Germany)	Re-examining the influence of a hydrogen termination together with an adsorbate layer from the atmosphere on the characteristics of the subsurface hole gas
A.3	Procopios Constantinou (London Centre for Nanotechnology, Great Britain)	Investigating the band structure of phosphorus delta-layers in Si(001)
A.4	Christof Dues (Universität Paderborn, Germany)	Ab-initio Investigation of Photocatalytic Water Splitting on LiNbO3
A.5	Niklas Fornefeld (Ruhr-Universität Bochum, Germany)	Adsorption on water-functionalized Si(001)-(2x1) surfaces

Poster B: "Nanowires and atomic wires" – Bonatz hall		
B.1	Anas Abdelwahab (Leibniz Universität Hannover, Germany)	Effective narrow ladder model for a correlated wire on a semiconducting substrate
B.2	Johannes Aprojanz (Leibniz Universität Hannover, Germany)	Electron Interference in Ballistic Graphene Nanoconstrictions
B.3	Jascha Bahlmann (Universität Osnabrück, Germany)	SPA-LEED investigations of quasi one dimensional Dysprosiumsilicide structures on Si(001)
B.4	Christian Braun (Universität Paderborn, Germany)	Au/Si(775) atomic scale nanowires: Structural, electronic, magnetic, and optical properties
B.5	Frederik Edler (Leibniz Universität Hannover, Germany)	Transport in atomic wires
B.6	Yasemin Ergün (Leibniz Universität Hannover, Germany)	Ginzburg-Landau-Langevin and Su-Schrieffer-Heeger theories for the phase transition of In/Si(111)
B.7	Kris Holtgrewe (University of Paderborn, Germany)	Density functional theory investigation of rare earth silicide nanowires
B.8	Andreas Lücke (University Paderborn, Germany)	Time-resolved bond strengths evolution during surface phase transitions calculated from first principles
B.9	Zamin Mamiyev (Leibniz Universität Hannover, Germany)	Modification of plasmons in metal induced atomic wires
B.10	Federico Raffone (Politecnico di Torino, Italy)	A New Theoretical Insight Into ZnO NWs Memristive Behavior
B.11	Mohammed Shabat (Islamic Oniversity of Gaza, Palestine)	Hybrid Transfer Method for waveguide structure solar cell
B.12	Abdul Samad Syed (University of Duisburg-Essen, Germany)	Analysis of the electronic and atomic structure of Pb/Si(557) by polarization dependent two-photon photoemission

Poster C: "Interfaces" – Bonatz hall		
C.1	Iciar Arnay Ortigosa (Instituto de Ciencia de Materiales de Madrid, Spain)	Structural, electronic and magnetic characterization of Fe3O4/SiO2/Si heterostructures
C.2	Volodymyr Dzhagan (Chemnitz University of Technology, Germany)	Morphology-induced phonon spectra of CdSe/CdS nanoplatelets
C.3	Dominic Gerlach (Nat. Inst. for Materials Science, Tsukuba, Japan)	Characterization of buried metal/GaN interfaces
C.4	Jean Geurts (University Würzburg, Germany)	Surface Raman spectroscopy and first-principles calculations of the vibrational modes of the Au-(√3x√3)/Si(111) reconstruction
C.5	Christian Klump (Ruhr-Universität Bochum, Germany)	Magnetic and Structural Investigations of Ferromagnetic Nanostructures on GaAs Substrates
C.6	Julian Koch (Leibniz Universität Hannover, Germany)	Structural analysis of Ba2SiO4 thin films grown on Si(100)
C.7	Eric Mattson (University of Texas at Dallas, USA)	Structural Evolution of Hafnium Methacrylate Nanocluster Photoresists following Electron Beam Irradiation from in situ IR Spectroscopy
C.8	Gerson Mette (Philipps-Universität Marburg, Germany)	Charge transfer dynamics at the buried GaP/Si(001) interface studied by means of time-resolved SHG
C.9	Vissarion Mikhelashvili (Technion Israel Institute of Technology, Israel)	Negative Capacitance in Optically Sensitive Metal-Insulator-Semiconductor-Metal Structures on Silicon-on-Insulator
C.10	Vissarion Mikhelashvili (Technion Israel Institute of Technology, Israel)	Photo Sensitive Metal-Insulator-Metal Like Capacitor on Silicon with SrFeO-F Nano Particles Embedded in the Insulator Stack
C.11	Jill A. Miwa (Aarhus University,Denmark)	Engineering ultra-sharp, ultra-dense doping profiles in silicon: conduction and valence band quantization
C.12	Sergej Neufeld (Universität Paderborn, Germany)	Frequency shifts and Raman signatures at ferroelectric domain interfaces of LiNbO3 and LiTaO3 modeled by first principles
C.13	Oleksandr Selyshchev (Chemnitz University of Technology, Germany)	Electronic interaction between CdTe quantum dots and PEDOT:PSS: a photoluminescence quenching study
C.14	Ercan Şener (Anadolu University, Turkey)	Investigation of the effects of different post-annealing conditions on the electrical, structural and optical properties of vanadium oxide thin films
C.15	Ljupka Stojčevska Malbašić (University of Duisburg Essen, Germany)	Study of the photoinduced hidden state in 1T-TaS2 single crystals doped with selenium by means of time-resolved photoemission spectroscopy
C.16	Aliaksei Vetushka (Czech Academy of Sciences, Prague, Czech Republic)	Self-Assembled Monolayers of Oriented Dipoles as a Tool for Altering of Semiconductor Interfaces

Poster D: “2D materials and thin films” – Bonatz hall		
D.1	Yuriy Azhniuk (Institute of Electron Physics UNAS, Ukraine)	Laser-induced transformations in cadmium-doped As2S3 films
D.2	Timur Biktagirov (Universität Paderborn, Germany)	Defect-induced strain broadening of the infrared zero-phonon line of the NV- center in diamond
D.3	Alexander Chaika (ISSP, Chernogolovka, Russia)	STM visualization of surface and subsurface atomic structure of Gd3Si5/Si(111) using clean and oxygen-terminated tungsten tips
~~D.4~~		
D.5	Ayami Hattori (Nagoya University, Japan)	Feasibility study on topological quantum field effect transistor of silicene, germanene and stanene nanoribbons with edge hydrogen termination
D.6	Philipp Kröger (Leibniz Universität Hannover, Germany)	Transport of Top and Bottom Surface States in Ultra-Thin Bismuth Films
D.7	Ching-Shun Ku (National Synchrotron Radiation Research Center, Hsinchu, Taiwan)	Scanning Laue X-ray Nanodiffraction for Microstructural Imaging and Its Applications for Detecting Crystal Structure of 2D Materials
D.8	Jinwon Lee (Center for Artificial Low Dimensional Electronic Systems, Pohang, Korea)	Direct measurement of the excitonic energy gap of Ta2NiSe5 single crystal
~~D.9~~		
D.10	Johannes Reimann (Philipps-Universität Marburg, Germany)	Optical control of ultrafast currents in the topological surface state of Sb2Te3
D.11	Sergii Sologub (National Academy of Sciences of Ukraine)	Scattering of surface state carriers in Bi(111) nanofilms, grown on Si(111) by Pb and Sb adatoms
D.12	Daria Sostina (St. Petersburg State University, Russia)	Surface and bulk magnetic gapping in the electronic structure of (V, Fe, Mn) doped BiTeI.

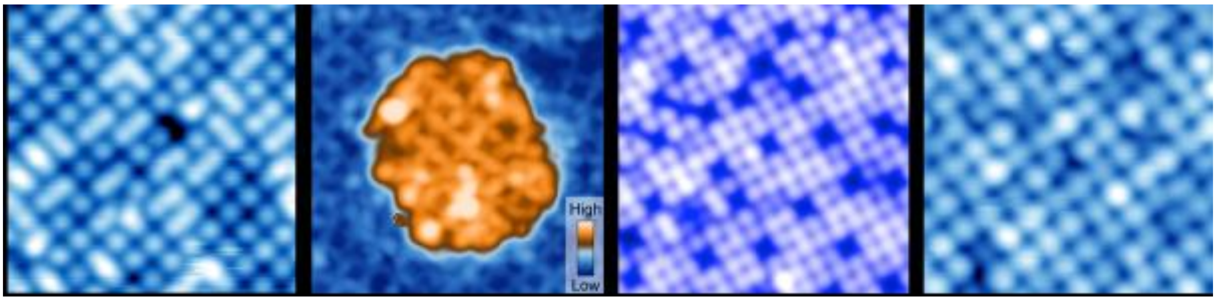
Abstracts

Atomistic understandings of perovskite oxide surfaces using scanning tunneling microscopy

Taro Hitosugi

School of Materials and Chemical Technology, Tokyo Institute of Technology

Two-dimensional electronic states formed at the surfaces and interfaces of complex transition-metal oxides have been promising platforms for exploring novel phenomena beyond bulk properties, such as high mobility electrons, superconductivity, magnetism, and topological phases. While establishing the microscopic mechanism is a critical factor for the further exploration of yet undiscovered quantum phenomena, understandings of atomic and electronic structures are still in its infancy. In this study, using scanning tunneling microscopy, we investigated the electronic structures of perovskite oxides, SrTiO3, LaAlO3/SrTiO3, SrVO3, La0.7Ca0.3MnO3 (Figure) Such surfaces exhibit a variety of properties including metal-to-insulator transition and coherent 2D states on surfaces. In addition, we have recently succeeded in the observation of atomic images on a LiTi2O4 superconductor. Here, we review the past, and present situation of the understandings of complex oxide surfaces1)-10), and discuss the future of oxide research.



$SrTiO_3$ substrate/film

$LaAlO_3/SrTiO_3$

$SrVO_3$ film

$La_{0.7}Ca_{0.3}MnO_3$ film

Figure: Examples of STM images on a variety of perovskite oxide surfaces.

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3) R. Shimizu, Hitosugi *et al.*, ACS Nano, 5, 7967 (2011).
4) R.Shimizu, Hitosugi *et al.*, Appl. Phys. Lett. 100, 263106 (2012).
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6) T. Ohsawa, Hitosugi *et al.*, ACS Nano, 8, 2223 (2014).
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Coherent quantum phenomena in superconducting atomic monolayers Pb/Si(111): A STM study

Dimitri Roditchev[1]

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In 1964 V. L. Ginzburg predicted that new superconducting phases could appear in ultrathin films deposited on insulating surfaces. In 2010 superconductivity below 2K was discovered in some crystalline atomic monolayers of Pb grown on atomically clean Si(111) [1,2]. Though, the amorphous Pb monolayer was found non-superconducting, but rather a correlated metal. Interestingly, Pb-monolayers can be on-demand made amorphous or crystalline, with or without presence of bulky superconducting Pb-nano-islands. This makes the Pb/Si(111) system useful to probe superconducting correlations in the vicinity of S-N or S-S' interfaces by STM [3,4].

When two superconducting Pb-islands are linked together by a few nanometer wide non-superconducting amorphous atomic layer of Pb, superconducting correlations may propagate between the two islands, allowing a dissipation-less Josephson current to flow through the link. In the presence of a magnetic field, the Josephson vortices are expected to appear in such S-N-S Josephson junction. Josephson vortices are conceptual blocks of advanced quantum devices such as coherent terahertz generators or qubits for quantum computing, in which on-demand generation and control is crucial.

In our lecture we describe a series of recent experiments which mapped superconducting correlations in the vicinity of S-N junctions [3,4] as well as inside SNS proximity Josephson junctions using scanning tunneling microscopy [5]. By following the Josephson vortex formation and evolution we demonstrate that they originate from quantum interference of Andreev quasiparticles, and that the phase portraits of the two superconducting quantum condensates at edges of the junction decide their generation, shape, spatial extent and arrangement [5].

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From Majorana bound states to topological quantum computation

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Abstract:

Semiconductor quantum wires proximity coupled to superconductors have become the material of choice to realize Majorana bound states. Recent experimental as well as material-science progress has intensified the search for implementations of topological quantum computation. In this talk, I will sketch recent ideas to realize quantum error correction on the basis of wire networks. Specifically, I will argue that color codes provide a natural setting in which advantages offered by topological hardware can be combined with those arising from topological error-correcting software [*]. Most importantly, color codes have a set of transversal gates which coincides with the set of topologically protected gates in Majorana-based systems, namely the Clifford gates. We illustrate the scheme by providing a complete description of a possible architecture.

References:

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Atomic-Layer Superconductors

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One or two atomic layers grown on crystal surfaces are recently found to be superconducting: a monolayer of Pb [1,2,3], two atomic layers of In [1,2], Ga [4], and Tl [9], and a monolayer of Tl+Pb alloy [5] on Si(111) surface, a single unit layer of FeSe [6,7] film, Ca-intercalated double-layer graphene [8], and so on. Interesting issues of these 'atomic-layer superconductors' may be three fold; (1) Large fluctuation due to the two-dimensionality (2D), (2) Influence of the substrate, and (3) symmetry breaking.

(1) Large fluctuation due to 2D: According to Mermin-Wagner Theorem, 2D lattices do not have phase transitions due to large fluctuation. This means no superconductivity in monatomic layers. But in reality, because of the 'quasi-2D' nature, superconductivity occurs even in monatomic layers. Then, we can expect phenomena due to large fluctuation such as Aslamazov-Larkin- Maki-Thompson corrections due to the amplitude fluctuation, and Berezinskii-Kosterlitz- Thouless (BKT) transitions and a Bose metal phase [9] due to phase fluctuation.

(2) Influence of substrate: The superconducting transition temperatures T_C of most of the known atomic-layer superconductors are lower than those of the bulk materials. One exception is the single unit-layer FeSe film which shows T_C higher than 100 K while that of the bulk FeSe crystal is a few K [6,7]. Possible explanations for this is interface phonons and charge transfer from the substrate. This example indicates possibility to enhance T_C by making materials as thin as monolayer thick on suitable substrates.

(3) Symmetry breaking: Since the material surfaces are in a situation of break-down of space-inversion symmetry, spin degeneracy in electronic states can be lifted (Rashba effect) [5]. Superconductivity at surfaces and monolayers are then novel because singlet- and triplet- Coopers can be mixed (parity-broken superconductivity). Actually, scanning tunneling spectra taken from the superconducting (Tl+Pb) monolayer on Si(111) which showed Rashba effect simultaneously, was not reproduced by BCS theory based on *s*-wave superconductivity. The spectra was instead well reproduced by assuming an anisotropic gap function. Furthermore, a pseudo-gap structure was found in STS beyond the upper critical field and at the vortex core in this system. This may be a sign of a new type of superconductivity.

In my talk I will show some experimental data of *in situ* four-point probe transport measurements and ultra-low temperature scanning tunneling microscopy/spectroscopy on some atomic-layer superconductors, and discuss the future. This work is based on collaboration with the groups of A. A. Saranin, A. V. Zotov in Russia, and Y. Hasegawa at ISSP of Univ. Tokyo.

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Majorana Fermion in the Vortex of Topological Superconductors by proximity effects

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In this talk, I will discuss our recent efforts to make artificial topological superconductors by proximity effects and identify the Majorana fermion (MF) in the vortex core [1-4]. As predicted, MF in the vortex of topological superconductor appears as a zero energy mode with a cone like spatial distribution. Also, MF can induce spin selective Andreev reflection (SSAR), a novel magnetic property which can be used to detect the MFs. Here, all the three features are observed for the MFs inside vortices in $Bi_2Te_3/NbSe_2$ hetero-structure [2-4]. More importantly, all evidences are self-consistent. Our work provides definitive evidences of MFs and will stimulate the MFs research on their novel physical properties, hence a step towards their statistics and application in quantum computing.

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Giant In-plane Critical Fields of Superconducting Atomic Layers on Silicon

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State-of-the-art nanotechnology has now enabled the creation of two-dimensional (2D) superconductors with truly atomic-scale thicknesses: atomic layers epitaxially grown on substrate surfaces, atomic sheets such as intercalated graphene and transition-metal dichacogenides, superconductivity induced at interfaces, etc [1]. Intriguing phenomena and physics arising from the ideal two-dimensionality and the interface effects have made these materials very attractive. Of particular interest are epitaxially grown elemental-metal atomic layers on semiconductor surfaces [3,4], which feature unique atomic structures and electronic states as well as high crystallinity. This class of 2D superconductors can be strongly influenced by the Rashba effects due to the spin-orbit interaction and the space inversion symmetry breaking at the surface [5], and may be further modified through charge and spin doping using adsorption of organic molecules [6]. In this presentation, we report on magneto-transport measurements of the indium atomic layers on silicon, i.e. the Si(111)-($\sqrt{7}\times\sqrt{3}$)-In surface. The experiments were conducted in a home-developed ultrahigh-vacuum compatible electron-transport-measurement system with the lowest sample temperature of 900 mK and the largest magnetic field of 5 T. We found that the superconductivity is highly robust when a magnetic field was applied to the sample in an in-plane direction. The in-plane critical field extrapolated toward zero temperature was 15-20 T, which was 3-4 times larger than the Pauli limit field of B_P = 5.6 T corresponding to T_c = 3 K. The possible influence of the Rashba effect will be discussed based on a spin-split Fermi surface of this atomic layer superconductor.

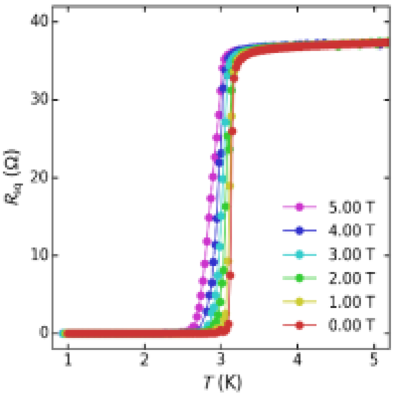

Fig. 1 Superconducting transitions of the Si(111)-($\sqrt{7}\times\sqrt{3}$)-In surface under in-plane magnetic fields.

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Characterizing buried nano-interfaces in nanocrystal solids at the atomistic level: a coupled theoretical-experimental approach

E. Scalise (1), D. Talapin (2), G. Galli (2), S. Wippermann (1)

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(2) Institute for Molecular Engineering, U Chicago

Nanocrystal-solids (NC-solids) and novel Silicon phases offer exciting prospects to create materials, which are non-toxic and earth-abundant, with properties tailored precisely towards solar energy conversion or electronic applications. Recent experimental advances demonstrate the synthesis of fully inorganic nanocrystal-solids from scalable and cost-effective wet chemical solution processing. However, the properties of these nanomaterials are dominated by their large surface to volume ratio. Detailed knowledge of the nanoscale surface chemistry is required to enable rational device design. Surface ligands that bind to the NC surface and out of which the embedding matrix is eventually formed are an integral part of NC-solids. By combining electronic structure calculations of surfaces with experiments and first principles molecular dynamics for NC-solids, we show that both the nanocrystal-matrix interface and the matrix itself form complex structural motifs, depending on specific synthesis conditions. The structural and electronic properties of the resulting nanocomposite point at the key role of the matrix in enabling efficient electronic transport, and at important modifications of embedded NCs with respect to isolated ones.

GaP/Si(001) polar-on-nonpolar epitaxial growth revisited by scanning tunneling microscopy

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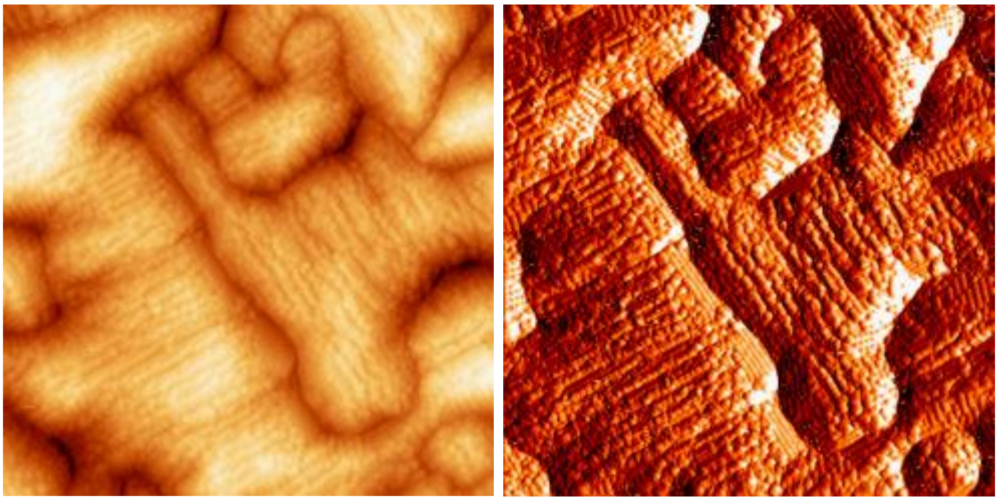
[3] Birla Institute of Technology and Science, Pilani, India

The monolithic integration of III-V based laser sources on a silicon chip requires avoiding/limiting the formation of antiphase disorder at the polar-on-nonpolar III-V/Si interface [1]. We present here a detailed scanning tunneling microscopy (STM) study of epitaxial GaP layers grown by molecular beam epitaxy (MBE) [2] on nominal and vicinal Si(001) substrates for photonic applications. The surface morphology of GaP films with thickness varying between 3 and 220 nm is investigated from large scale down to the atomic level. We show that the use of vicinal Si(001) substrates presenting bi-atomic steps only promotes growth of a dominant polarity at the early deposition stages, allowing the complete annihilation of the antiphase boundaries (APBs) for thicker GaP films. From atomically resolved STM images, we also observe that the terminal GaP facets at the early growth stages are strongly modified by the use of a vicinal Si(001) substrate. Based on these STM observations, the three-dimensional GaP/Si(001) MBE growth mode is discussed in terms of surface/interface energies computed by ab-initio calculations. This study gives new ideas on the effect of a controlled substrate miscut on APBs formation and annihilation mechanisms.

This work is supported by the French National Research Agency project ANTIPODE (Grant no. 14-CE26-0014-01), Région Bretagne and Rennes Métropole.



*(60*60)nm^2 STM image (left : topography, right : current error) of antiphase domain morphology for a 10nm thick GaP epilayer grown on nominal Si(001) surface. (001), (136), (113) and (114) terminal GaP facets are observed.*

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Towards atomic-scale switches based on self-assembled magic clusters

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Atomic-scale switches represent the ultimate level of device miniaturization. The possibility to realize switches with sizes down to the level of single atoms using a scanning tunneling microsope (STM) has been demonstrated already over 2 decades ago [1]. In the meantime, atomic scale switching was also demonstrated on surfaces of silicon [2,3], the most technologically relevant semiconductor. However, the practical application of these switches is still limited by two main obstacles. First, most of the switches realized up to now only operate at cryogenic temperatures and second, they are constructed using STM based atomic manipulation being an extremely slow fabrication method.

In this work, a bistable switching behavior at room temperature is observed for small clusters growing in a self-assembled way on the Si(111)7×7 surface after deposition of the trivalent rare-earth metals Tb and Dy at moderate temperatures. The self-assembled growth method allows to grow extremely high cluster densities within minutes, making these clusters in principle very interesting for applications, e.g. as high-density memory devices. Here, the Si(111)7×7 reconstruction is used as a template to grow identical, so-called magic clusters within single 7×7 half unit cells. At appropriate growth conditions, rare-earth silicide clusters consisting of three rare-earth atoms and three silicon atoms are formed. While the clusters appear as symmetric triangles with respect to the underlying 7×7 substrate in filled states STM images, they appear rotated in empty states images leading to two possible cluster configurations. At appropriate tunneling conditions with the STM tip approached relatively close to the surface, a switching of the clusters between these two configurations occurs, while no switching is observed at larger tip-sample separations. Thus, the energy barrier separating the two configurations is high enough to suppress a thermally activated switching at room temperature, but increased tip-sample interactions can lead to a lowering of the barrier height and the observed switching behavior.

This work was funded by the DFG through FOR 1282 project D.

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Excitonic emission of hybrid lead iodide perovskite single crystals

E. Deleporte [a], H. Diab [a] , G. Trippé-Allard [a], F. Lédée [a,b] , G. Bouchez [c] , C. Vilard [c] , V.L.R. Jacques [d], A. Tejeda [d] , P. Audebert[b] , J.-S. Lauret [a] , D. Garrot [c]

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Since 2012, the 3D Hybrid Organic Perovskites of formula $CH_3NH_3PbI_3$ and their derivatives represent a "material breakthrough" for photovoltaïcs: in only 3 years, the efficiency of 3D HOP-based solar cells has progressed from 12% to more than 20%. These HOP molecules appear also very attractive for light-emitting devices such as electroluminescent diodes and lasers. Improvement of the performance of perovskite solar cells and optoelectronic devices may benefit from a better understanding of the intrinsic photophysics of materials. However, the properties of films are very dependent of the grain structure. We will focus here on the synthesis of HOP single crystals and we will study their optical properties. Figure 1 shows a millimetric $CH_3NH_3PbI_3$ single crystal, whose optical properties are compared to those of thin polycrystalline films. In particular, the main feature in single crystals is the appearance, in the low temperature luminescence spectra, of a sharp emission line (FWHM ~ 5 meV) at high energy which is attributed to the free exciton signature (figure 1). Experiments performed as a function of temperature confirm the existence of a strong electron-phonon coupling. We highlight the extremely high stability of the single crystals compared to the thin layers: defects and grain boundaries are then thought to play an important role in the degradation mechanism.

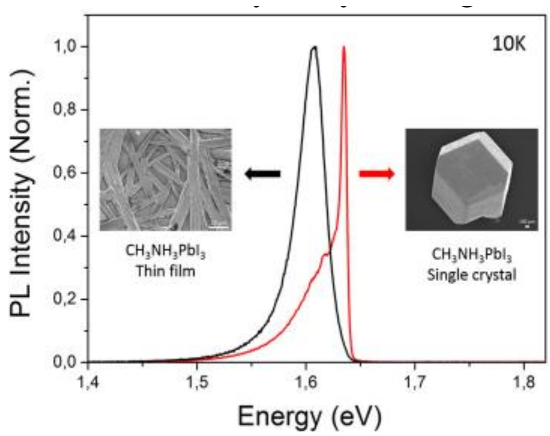

Figure 1 Photoluminescence spectra of $CH_3NH_3PbI_3$ thin film (black) and crystal (red) at 10K.

Acknowledgements

The project leading to this application has received funding from the European Union's Horizon 2020 programme, through a FET Open research and innovation action under grant agreement No 687008

Effect of β-diketone passivation on solution processed zinc oxide nano-layers used in thin film transistors

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Solution processed metal-oxide thin film transistors are used in optical, mechanical and electrical applications. Oxygen and moisture induced surface traps cause instability and unreliability under electrical operation. For application purposes it is necessary to passivate surface traps. To achieve this goal it is of great interest to investigate surface properties and trap mechanisms.

In this work thin film transistors were fabricated by depositing ZnO thin films with a thickness of 12 nm by spray pyrolysis on substrates with predefined electrodes. Because of their instability against oxygen and moisture the thin film transistors were passivated using for this purpose tailor made β-diketones with trifluormethyl and benzene-derivatives as substituents. After passivation of the ZnO surface transistors exhibit reduced hysteresis, increased mobility and better stability against electrical bias stress. The improvement of ZnO thin film transistors depends on used passivation molecule and exposure time. UV-Vis, AFM and IV measurements were used to characterize optical, morphological and electrical properties, respectively. We conclude that functionalized β-diketones passivate surface traps on solution processed ZnO thin films achieving better stability against oxygen and moisture under electrical operation.

Porous silicon distributed Bragg reflector-Au nanocavity based dual sensing structures

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Hybrid photonic-plasmonic systems are emerging in fields requiring a specific modulation of light behaviour, such as optoelectronic and biosensing devices. In this frame, photonic-plasmonic systems have been created by combining porous silicon (PSi) based distributed Bragg reflectors with arrays of Au nanocavities. PSi multilayer stacks were produced by cyclic current driven electrochemical etching of p-type monocrystalline silicon wafers, which led to contrasting porosity strata and to a selective interferential response [1]. On top of this structure, a plasmonic surface consisting of Au nanocavity arrays was obtained by a process based on a sequence of formation of a polymer layer on the PSi surface, decoration with large area colloidal monolayers, shaping with reactive ion etching, deposition of a 200 nm thick Au layer and a final step of lift off of the remaining colloidal structure [2]. Different post-processing treatments of annealing and chemical etching have been applied to modify the Au microstructure. The dual structures have been characterized by scanning electron microscopy, which has allowed to infer the main characteristics of the dual system, such as thickness of individual PSi layers and evolution of the grain size of the Au out-structure. Moreover, process cumulative reflectance measurements allowed evaluating the individualized optical contributions and their coupling (Figure 1). The results show that an increase of the sensitivity of a potential sensing device is obtained when comparing the reflectance drop at circa 750 nm….

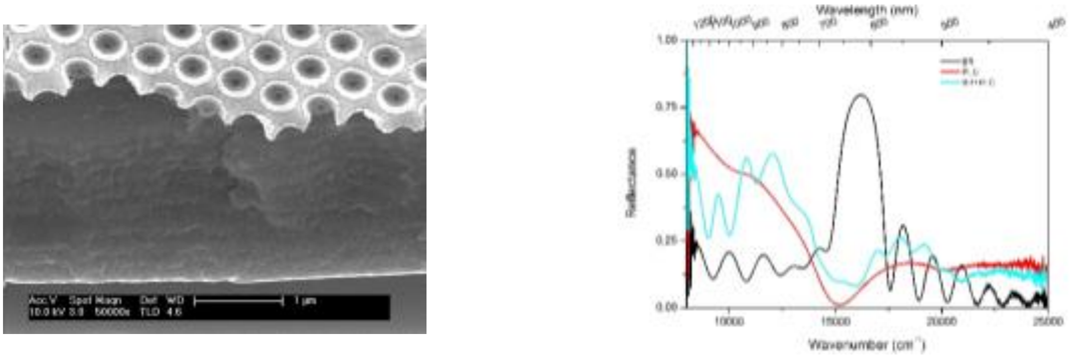

Figure 1: SEM image of the hybrid system (left). Optical characterization of the Bragg reflector (BR, black), plasmonic surface (PLC, red) and hybrid system (BR+PLC, light blue) (right).

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New Instrumentation for spin-integrated and spin-resolved Momentum microscopy – METIS and KREIOS

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Two new momentum microscopes are presented by SPECS: our newly developed time-of-flight momentum microscope METIS and the energy dispersive and filtered momentum microscope KREIOS. Both are using an optimized lens design which provides simultaneously highest energy, angular and lateral resolution. The lens provides a full 2π solid acceptance angle with highest angular resolution. in contrast to standard ARPES measurements with conventional hemispherical analyzers, electronic structure data from and beyond the 1st Brillouin zone is recorded without any sample movement. In addition the lens of such an instrument can work in a lateral imaging mode for microscopy as well. This enables navigation on the sample and reduces the size of the area under investigation in ARPES down to a few micrometers in diameter. This combination of large acceptance angle, high angular resolution and small acceptance area, makes this instrument the ideal tool for electronic structure studies on small samples or sample areas. the design is compact with a straight optical axis. Operation modes are (k_x,k_y,E_k) data acquisition by operation in energy filtered k-space imaging, (ToF-)PEEM mode, energy-filtered real space imaging and micro-spectroscopy mode.

The 3D (k_x, k_y, E_k) data recording is done with a 2-dimensional delayline detector, with a time resolution of 150 ps and count rates up to 8 Mcps. It uses channelplates with 40 μm spatial resolution. While the x,y position of an incoming electron is converted into k_x,k_y wave vector, the kinetic energy E_k is determined from the flight time t in METIS or obtained directly by the energy filter in KREIOS. Spin-resolved imaging is achieved by electron reflection at a W(100) spin-filter crystal prior to the 2-dimensional delayline detector. Electrons are reflected in the [010] azimuth at 45° reflection angle. Varying the scattering energy one can choose positive, negative, or vanishing reflection asymmetry.

Besides a description on how the instruments work data from both instruments on different single crystalline materials will be presented.

Magnetic interactions in artificially created Mn assemblies in a GaAs (110) surface

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We have used Scanning Tunneling Microscopy (STM) to create and study the electronic properties of dedicated assemblies of magnetic atoms in a semiconductor surface. Several STM manipulation approaches have been tested to get the best control over the manipulation of Mn atoms on the 110-surface of GaAs. The best manipulation approach has been used to create pairs, trimers, and tretramers of Mn atoms embedded in the surface layer of GaAs, see fig 1. We have used spectroscopic techniques to determine the electronic interactions between the magnetic Mn atoms in these artificially created assemblies. The electronic interaction, which is strongly affected by the magnetic interactions between the Mn atoms, is found to be highly anisotropic. We observed a substantially magnetic coupling only for Mn pairs aligned in the [110] direction. This observation is in contrast with previous experimental results [1], where substantial Mn-Mn interaction has been reported for pairs in other directions. Our excellent energy and spatial resolution and the creation of more complex linear and non-linear assemblies allowed for a deeper analysis. We showed that the influence of the surface on the anisotropic Mn-Mn magnetic interaction is very important and correctly captured in the model presented in [2].

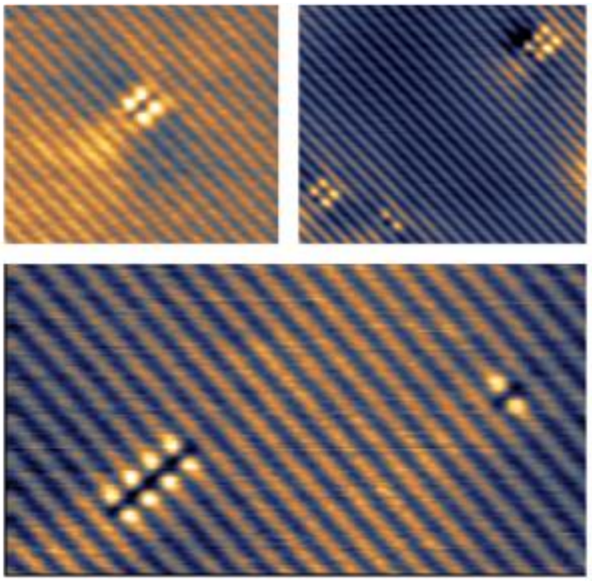

Fig. 1: Examples of Mn assemblies in the 110 surface of GaAs that have been created by STM manipulation.

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X-Ray reflectivity measurements of ultrathin layers in 2DEG AlGaN structures

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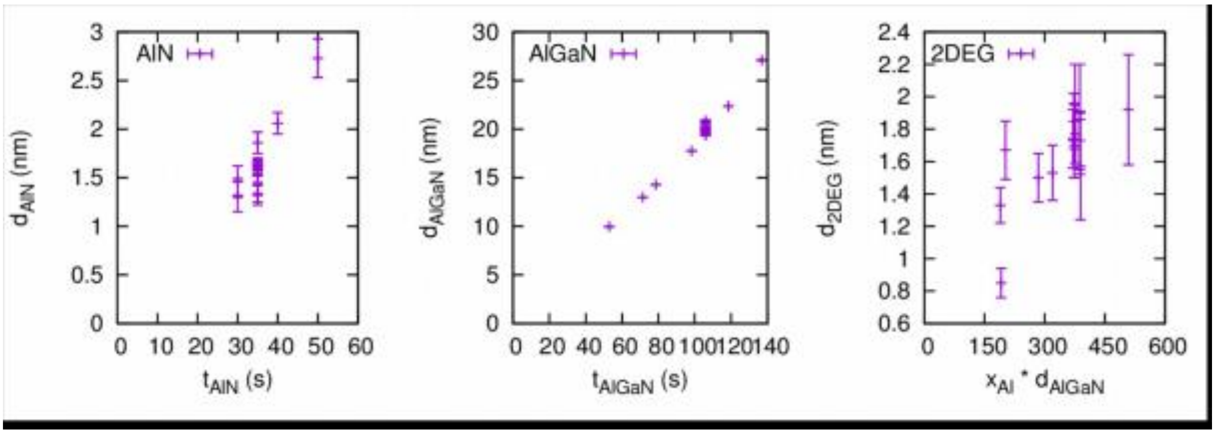
In order to optimize the mobility of 2DEG AlGaN/AlN/GaN structures we have grown a series of samples changing the Al-content and thickness of the different layers. The samples were grown in an Aixtron 200RF MOVPE using standard precursors. The samples under investigation consist of a 2 micron GaN buffer layer grown on c-oriented sapphire substrate followed by a thin AlN layer with varying thickness. The subsequent AlGaN layer was varied in thickness and Aluminum content. To understand the properties of 2DEG AlGaN/GaN structures precise knowledge of the structural properties is required. Therefore we have performed X-ray diffraction measurements. XRD measurements show well resolved thickness oscillations of the AlGaN layer which allows to determine the thickness of the AlGaN layer and the concentration. Reciprocal space maps reveal that the layers are grown pseudomorphically on the GaN buffer. While the AlGaN layer can be characterized easily, it is almost impossible to characterize the ultra thin AlN layer by XRD. In contrast to that X-ray reflectivity measurements can be sensitive to layer thicknesses below 1 nm. In order to characterize the AlN layer we have performed such XRR measurements. These measurements allow indeed to characterize the AlN layer, as shown in the figure. The thickness of the AlN and AlGaN layer depend linearly n t growth time, as expected. In order to describe the measured spectra we had to introduce two more layers. One is the usual oxidized surface layer which had a thickness of approximately 1nm, but there is an additional layer underneath the AlN. XRR is sensitive to the electron density this might be a signature of the 2DEG. As shown in the rightmost figure we observe a linear dependence of this layer thickness on the Aluminum content and the AlGaN layer thickness. Consequently it appears plausible that X-ray reflectivity is not only sensitive to material contrast but also to a local density enhancement induced by heterostructure design. Ultimately, one may even be able to determine the 2DEG electron carrier density using Xray measurements.



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Local deep level transient spectroscopy for two-dimensional MOS interface characterization based on scanning nonlinear dielectric microscopy

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[1] *Research Institute of Electrical Communication, Tohoku University*

Physical properties of metal-oxide-semiconductor (MOS) interface are critical for semiconductor devices. There are several techniques for characterizing MOS interface properties. Deep level transient spectroscopy (DLTS) [1] is one of powerful techniques capable of macroscopic quantitative evaluation of trap density at/near MOS interface. But it is easily imagined that actual trap is not homogeneously distributed but has two dimensional distributions in atomic scale and even in mesoscopic scale. Therefore, it is very important to characterize MOS interface microscopically. Unfortunately, it is impossible to observe such inhomogeneity by using conventional macroscopic DLTS method. Moreover, in our best knowledge, SPM based two dimensional DLTS imaging has not been reported.

In this paper, a new technique for local DLTS imaging using scanning nonlinear dielectric microscopy (SNDM) [2] is proposed. This method enables us to observe two dimensional distribution of trap density at/near MOS interface and is demonstrated with oxidized SiC wafer.

We measured three n-type silicon face (4°-off) 4H-SiC wafer samples on which 45-nm-thick thermal silicon dioxide film was formed. Two of them were followed by post oxidation annealing (POA) in nitric oxide ambient with different annealing conditions: (a) 10 min in 1250°C and (b) 60 min in 1150°C. We labeled the samples without POA, with POA in condition (a) and with POA in condition (b) as #1, #2 and #3, respectively. These three samples were scanned on 1.5x1.5□m^2 square area with a resolution of 30x30 pixels and analyzed using the proposed local DLTS method (Fig.1). By analyzing the acquired images, time-constant and magnitude of transient capacitance response were obtained at each pixel. As shown in Fig.1, highest brightness was obtained from #1 and lowest one was obtained from #3, which is consistent with macroscopically obtained result (#1 sample has highest trap density and #3 sample has lowest one.). Furthermore, in the local DLTS images, we detected dark and bright areas, which can be translated as two dimensional trap distribution. This means that this is the first demonstrations of two dimensional imaging of trap distributions in MOS interfaces.

Thus, we conclude that this local DLTS technique can contribute to understanding of two dimensionally distributed microscopic physical properties of MOS interface.

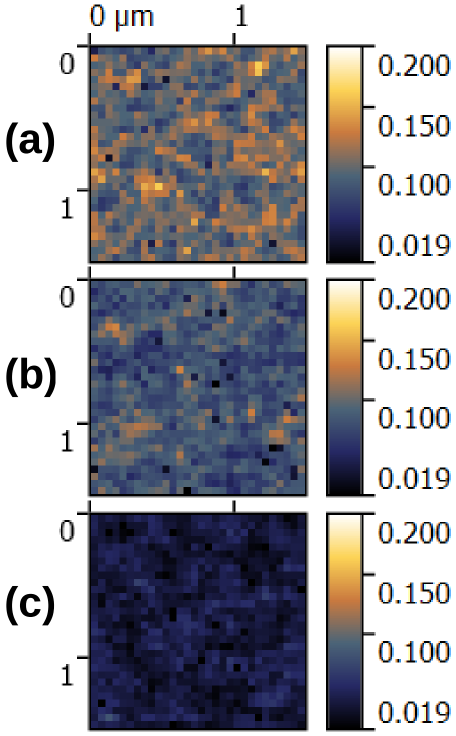

Fig. 1. Local-DLTS images of SiC MOS interfcae (a) sample #1, (b) #2 and (c) #3. The dark and bright areas are interpreted as low D_{it} (trap density) area and high D_{it} area, respectively.

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Electronic properties of the Fe/GaAs(110) interface

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In order to check the validity of theoretical models describing the microscopic process of Schottky barrier (SB) formation, the structural and electronic properties of Fe/GaAs(110) interfaces have been investigated by means of atomically resolved cross-sectional scanning tunneling microscopy (XSTM) and spectroscopy (XSTS) in combination with density functional theory. To yield an epitaxial and atomically flat interface without any sign of compound formation, the Fe/GaAs(110) interface was grown at low temperature and subsequently annealed to room temperature [1]. From XSTS measurements of the electronic landscape of the space charge region (SCR) of the Schottky contact, the bending of the valence and conduction band along the SCR for n- and p-type doped Fe/GaAs(110) interfaces is demonstrated. To properly interpret the XSTS data, the tip induced band bending has to be taken into consideration. This is addressed by means of a 3-dimensional finite element method (3D-FEM) calculation.

Atomically resolved XSTS measurements across the Schottky contact reveal a continuum of states in the band gap of the semiconductor in the first few atomic layers at the interface. For the n-type junction the metal-induced-gap-state model (MIGS) can explain the experimental data. For the p-type case, a combined MIGS and bond polarization model qualitatively explains the experimentally observed large SB height by taking into consideration the additional positive charge inside the valence band due to Fe-As hybridization that partially compensates the negative charge of the MIGS.

The influence of the film thickness as well as the growth conditions on the SB height were investigated. XSTM topographies indicate that e.g. Fe sub-monolayer pre-growth at room temperature has a significant impact on the atomic structure of the interface and increases the degree of intermixing, which also affects the Schottky barrier height.

Our approach yields a spatial and energetic map of the local density of states that covers both the band gap and the valence and conduction bands at the interface. In combination with density functional theory calculations this allows a better and deeper understanding of metal-induced gap states and bond polarization at the interface.

This work was supported by the DFG SPP 1285.

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Non-destructive imaging of atomically-thin nanostructures buried in silicon

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Semiconductor nanostructures consisting of areas of buried dopant atom(s) are crucial components for present and future CMOS transistor technologies as well as for emerging quantum computing architectures. Consequently, non-invasive imaging and electrical characterization of buried nanostructures, with precise lateral and depth resolution, would be of great value for the development and inspection of integrated circuits and quantum devices. I will describe the fabrication of three-dimensional (3D) phosphorus nanostructures fabricated via scanning tunnelling microscope-based lithography, and subsequent characterization with scanning microwave microscopy (SMM). The SMM measurements, which are completely non-destructive and sensitive to as few as 1900 to 4200 densely packed P atoms 4 to 15 nm below a silicon surface, yield electrical and geometric properties in agreement with those obtained from electrical transport and secondary ion mass spectroscopy (SIMS) for un-patterned phosphorus δ-layers containing ~1013 P atoms. The imaging resolution was 37±1 nm in the lateral and 4±1 nm in the vertical direction, both values depending on SMM tip size and depth of dopant layers. Our results open up exciting opportunities for dopant nanostructure fabrication by providing a measurement capability not possible with any other technique.

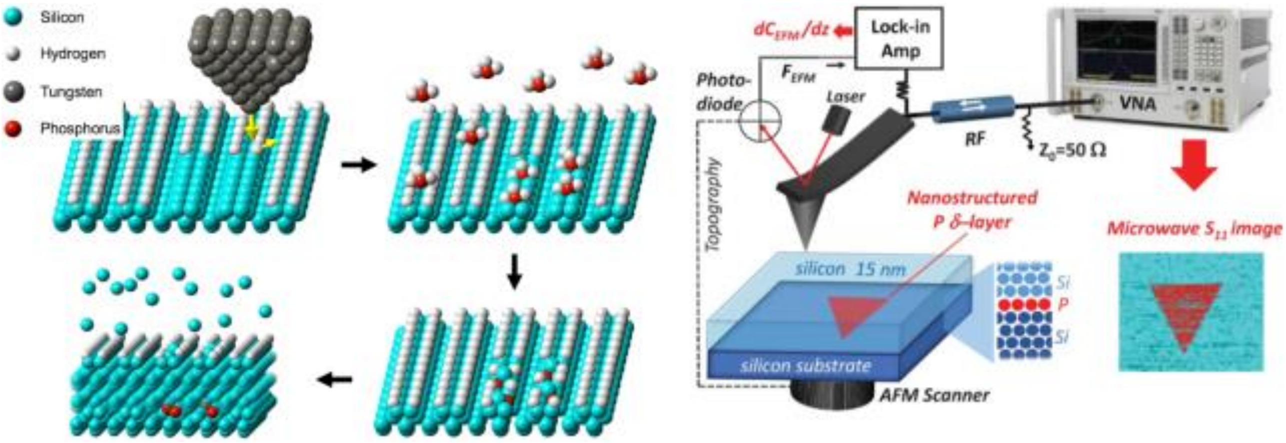

Figure: Hydrogen resist lithography process for fabricating buried dopant nanostructures (left). Scanning microwave microscope (SMM) experimental set-up (right).

Electronic structure of the non-polar GaN(1010) surface

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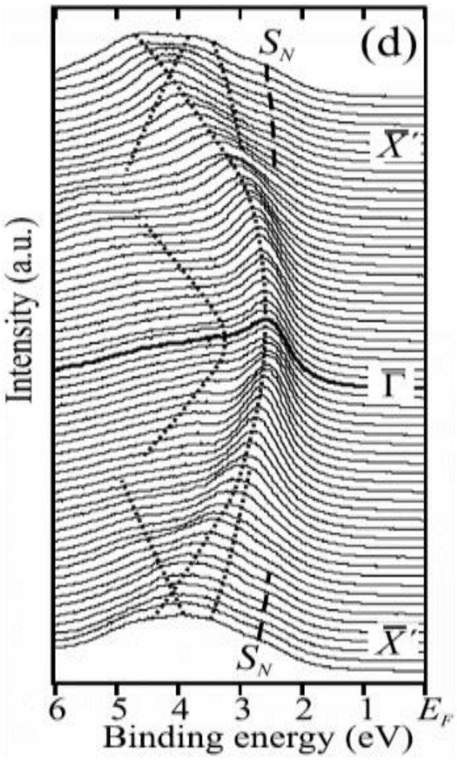
Wurtzite GaN as a direct wide-bandgap semiconductor is of extraordinary interest for optoelectronic applications [1]. Its non-polar GaN(101□0) surface, the so-called *m*-plane, plays an important role e. g. as the predominant sidewall facet of nanowires or as a promising growth substrate for a reduction of polarization fields in nitride devices [2,3]. However, the nature of the GaN(101□0) surface states is not well understood up to now: The electronic dispersions of the filled nitrogen-derived SN state and the empty gallium-derived SGa state have not been determined experimentally, and the energetic position in the GaN band gap of the latter is still a matter of debate [4,5].



In this work, we studied the electronic structure of the *n*-GaN(101□0) cleavage surface using angle-resolved and core-level photoelectron spectroscopy. An example for an angle-resolved spectra series taken in the Γ□−X'□ direction is shown in the figure, where the bulk valence bands (dotted) and the filled SN surface state band (dashed) are clearly identified. We determined the dispersion of the SN surface state band and derived the effective masses for both the bulk valence band and the SN surface state band. In addition, we determined the position of the Fermi level within the band gap to ~2.3 eV above the valence band minimum, corresponding to the energetic position of the minimum of the empty SGa surface state band, in nice agreement with recent theoretical results [5].

This work was supported by the Deutsche Forschungsgemeinschaft, Sfb 787, TP A4.

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Indium incorporation related 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 at low T_G of about 970K and less (measured by a thermocouple). At these conditions the incoming flux is larger or equal to the desorption rate. The data reveal desorption of indium and at least another loss mechanisms and possibly some reconfiguration of the surface (coverage) during and after TMI supply. Furthermore, indium remains on the surface and is partly incorporated when TMI is already switched off. Part of this indium stems from surfaces in the vicinity of the sample. But most of the indium originates from the sample surface. We believe that indium clusters are formed on the adlayer or/and at defect sites and that indium from these cluster feed the adlayer or desorb. Thus the sharpness of the upper interface of the quantum well critically depends on desorption rate given by T_G and amount of supplied indium i.e. TMI flux and quantum well growth time.

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Exotic 2D nanostructures of adsorbates on silicon

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Crystalline atomic layers on solid surfaces are composed typically of a single building block, unit cell which is copied and stacked together to form the entire two-dimensional crystal structure. In contrast, one-atomic-layer-thick Tl-Bi compounds on Si(111) display quite a different arrangement. It represents a set of quasi-periodic tiling structures that are built by three tiling elements as building blocks. Though the layer is lacking strict periodicity, it shows up as an ideally-packed tiling of basic elements without any skips or halting (Fig. 1).

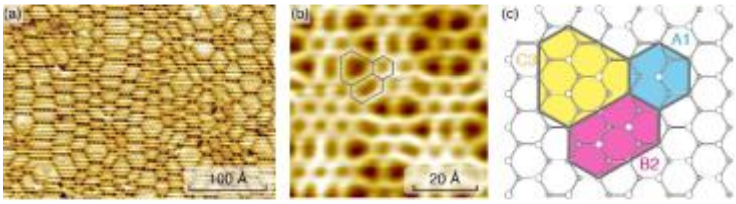

Fig.1. (a) STM image of the Tl-Bi surface and (b) its magnified fragment where three tiling elements are outlined. (c) Schematics illustrating the shape and size of the tiling elements, A1, B2 and C3.

When C_{60} fullerenes are adsorbed onto crystalline surface, one of two scenarios are typically realized. If fullerene-substrate interaction prevails over fullerene-fullerene interaction, fullerenes adsorb randomly on the surface. In case when fullerene-fullerene interaction dominates, close-packed C_{60} layers form. A very unusual behavior was detected for fullerene adsorption onto Tl/Si(111) surface. Fullerenes and Tl atoms form a composite molecular-atomic layer in which C60s are arranged into network which chains are filled by patches of Tl double-atom layer (Fig. 2).

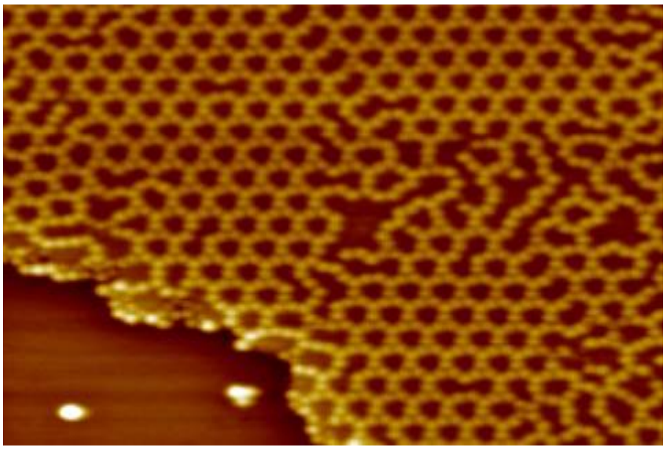

Fig.2. STM image of an ordered network built by C_{60} fullerenes upon deposition onto Tl/Si(111) surface.

The shown examples demonstrate possibility for growing exotic 2D materials on Si(111) surface via unusual growth mechanisms.

Interfacing Bragg Mirrors with Tilted Uniaxial Media: Exceptional Points and Chiral States

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The combination of a Bragg mirror with cylindrical symmetry and an uniaxial cavity material with its optic axis tilted against the growth direction represents an effectively biaxial optical metamaterial. Similar to the physics of biaxial crystals in the absorption regime [1,2,3], the dissipation in a transparent microcavity due to photon loss, manifested in finite mode broadening, leads to exceptional points and coalesced eigenstates as predicted in [4]. Our experimental investigation reveals already elliptically polarized states [3,5], proving our concept and opening the path to achieve optically chiral states without the presence of magnetic fields or ions and spin effects or spin-orbit coupling.

Via several design degrees of freedom regarding geometry and chemical composition, the spectral and angular positions of these chiral modes can be tailored. Possible applications arise from the use of such effects for circularly polarized emitters.

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Engineering the surface states of ZnO and SnO_2

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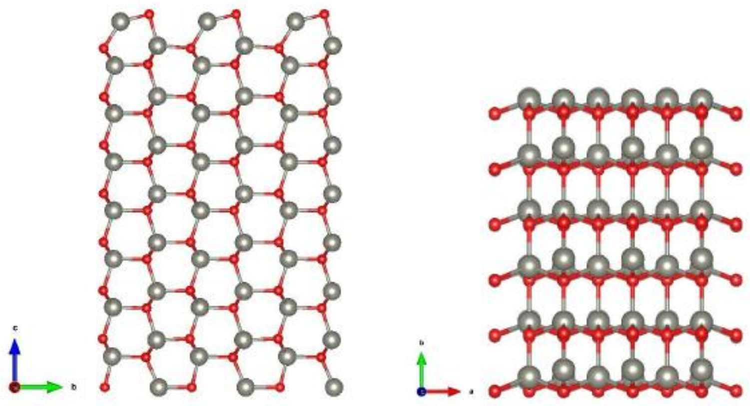
Inspired by experimental findings regarding the tunability of electron well states at zinc and tin oxide surfaces, we calculate the surface band structures for a range of surface slab models with different functionalisations. We perform density functional calculations and localize the atomic contributions of the surface atoms to identify the surface states, and the contribution of electron density from physisorbed or chemisorbed molecules.

We show a systematic modulation of the surface bands with the nature of the adsorbed molecules in all cases. We also discuss the differences between the different surface facets (1010, 11-20, and 1121) in the case of ZnO, as well as the differences observed for the more complex SnO_2 structure.



(a) Side view. (b) Top view.

Side and top view of the ZnO (1010) surface (16 x single layers, 32 atoms per unit cell) for one choice of termination studied. Gray = Zinc-atom, red = Oxygen-atom.

Ultrafast electron transfer across a ZnO-organic interface

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Combining organic molecules with inorganic semiconductors is a promising route towards novel optoelectronic devices, such as organic LEDs or photovoltaics [1]. The ability of electrons to cross the hybrid interface is a crucial factor for the efficiency of such devices. We investigate this fundamental process at the ZnO/5-phenyl-pyridine (5P-Py) surface using time-resolved two–photon photoelectron spectroscopy (2PPE). Time-resolved 2PPE is a unique tool to access both the occupied and unoccupied electronic states and their dynamics. We find that adsorption of 5P-Py (ca. 7 nm) on ZnO (10-10) leads to a substantial work function reduction and the formation of an occupied interfacial state close to the Fermi level. This state can be used as an initial state to populate the molecular LUMO without directly exciting the molecules. Subsequently, the LUMO population decays on a sub-100 femtosecond timescale, possibly by back-transfer to ZnO. If, on the contrary, the molecules are directly excited via HOMO-LUMO excitation, the LUMO population shows a picosecond lifetime. Our findings suggest that while electronic coupling across the interface is strong, the localization of electron and hole within the molecular layer slows down the electron transfer substantially.

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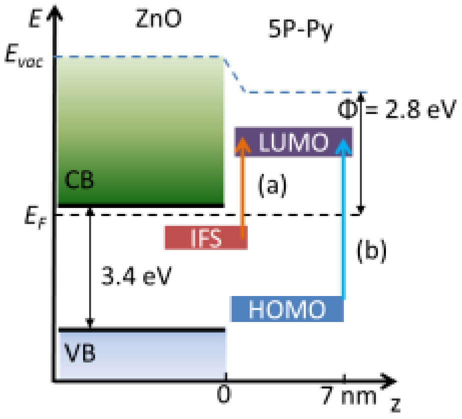

Fig. 1 Electronic Structure of ZnO/5P-Py indicating the two excitation pathways. (a) Excitation resonantly from the interfacial state (IFS) into the 5P-Py LUMO. (b) Excitation from the HOMO to the LUMO.

Photochromic phosphonic-acid diarylethene self-assembled monolayer switches on polar ZnO surfaces

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Photochromic molecular switches are attractive components in multifunctional devices, such as phototransistors and optical memories. By inserting a molecular switch interlayer into these devices, they can be used to modulate charge injection and transport by forming photoswitchable charge traps or charge barriers under the stimulation by external light.[1] In the photo-switching process, the photochromic switches undergo reversible changes of their frontier energy levels, which results in an increase or decrease in the energy level offset at the interface with inorganic semiconductors.

Here, we investigate the interfacial chemical and switching properties of the phosphonic-acid diarylethene (PA-DAE) switch in form of a self-assembled monolayer (SAM) on ZnO(0001) and ZnO(000-1) surfaces by photoelectron spectroscopy. The observed work function increase is attributed to the introduction of a surface dipole; the binding modes of the phosphonic-acid linker were retrieved from the deconvolution of core level (O 1s) spectra, indicating the formation of mixed bidentate and tridentate binding. The quantification of core level spectra supports to picture of a densely packed layer on both ZnO surfaces. Upon appropriate illumination with ultraviolet and visible light, respectively, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbitals (HOMO) level of the PA-DAE molecules, which in the further will be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

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Kinetic roughening study in electrodeposited films

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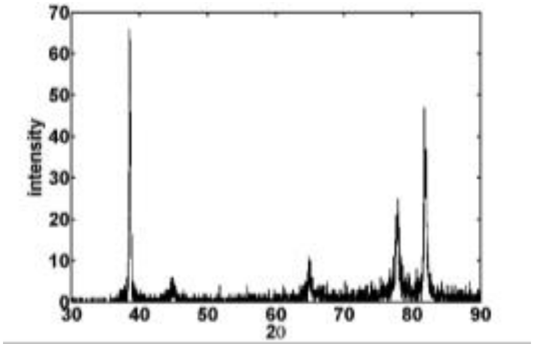
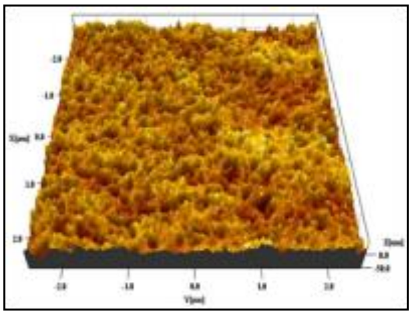
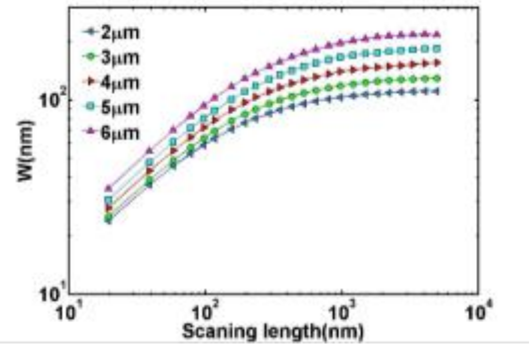
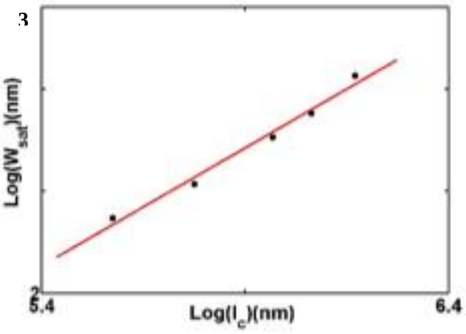
The morphology and roughness of different thin films have been studied using atomic force microscopy (AFM) and kinetic roughening calculation. Our films were grown on n-type Si substrates using non-expensive electrodeposition technique. The average crystalline size of the film surfaces is calculated from X-ray line broadening using (111) peak and Debye–Scherrer formula. The surface morphology was evaluated by image analysis methods based on atomic force microscopy micrographs. It was found that electrodeposited silver films, the surface roughness increases with increasing the film thickness. The data also consist with a complex behavior which is called as anomalous scaling. Scaling laws analysis for Ag films presents two distinct dynamics including large local and scale roughness and shows a power law dependency on the thickness of silver film. The values of Hurst exponent H and growth exponent β that measured by us are close to a conservative deposition process. It suggests that surface-diffusion plays a dominant role. The results indicate that grain size and morphology of samples can easily be controlled by using different thickness.









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Manipulation of 2D states on the surfaces of transition metal oxides

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The study of two-dimensional states formed at the interface between two insulating transition metal oxides, or at the interface of such a system with vacuum, has in the last decade developed into a research field of its own. One of the prime reasons is the extremely rich phase diagram of this class of materials. This includes varied magnetic order, strong spin-orbit interaction, ferroelectricity, and superconductivity. Furthermore, combinations of materials can be grown with atomic layer precision and most of the applied techniques are easily scalable. Moreover, the large band gap and low intrinsic doping of most transition metal oxides makes sure that the 2D electron states form the main contribution to the transport properties and allow for tunable properties by gating.

Although the field is driven by state-of-the-art transport experiments, angle-resolved photoemission spectroscopy (ARPES) experiments have played a significant role to elucidate the nature of the states especially at surfaces. Significant progress is made in using soft X-ray photon energies to probe states at a buried interface, but at these high energies the cross section of strongly localized 2D states is very low, hindering high resolution measurements.

Here we will show also states at clean surfaces of transition metal oxides in the $XTiO_3$ (X=Ca, Sr, Ba) phase diagram can be controlled and the results can be observed by high resolution ARPES. We will show how bulk ferroelectricity influences the states at the surface and in thin film overlayers. Furthermore, we will use the stoichiometry and surface structure to tune the carrier density and dimensionality of the states. Moreover, it will be shown how the crystal and electronic structure influence the Rashba-type spin-orbit splitting in these systems.

Phonon Mediated Optical Stark Effect for Hybrid Heterostructures

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Phonon mediated optical Stark effect for organic-semiconductor heterostructures (quantum well, system of quantum dots) with existence of hybrid Wannier-Frenkel excitons will be studied theoretically, taking into account in the macroscopic phonoriton equations the two-component exciton state. The phonoriton quasi-eigenstate, which have been introduced theoretically and observed experimentally previously, characterizes a coherent superposition of exciton, photon and photon. The spectrum arises from mutual hybridization and unification of the initial excitonic polariton and phonon dispersion.

Wannier-Frenkel hybrid exciton state, which exists at the interface of organic-inorganic systems, has optical and electronic properties greatly different from both Wannier and Frenkel excitons and can overcome the limitation of each kind of excitons. A hybrid Wannier-Frenkel exciton is currently considered as one of the most promising electronic states that can be implemented in optoelectronic devices of a new generation.

The system of macroscopic equations of hybrid excitons, photons and phonon is investigated in order to model the optical Stark effect for the hybrid systems with combination of semiconductor and organic materials. While the Frenkel exciton component has a strong coupling with the light field (polariton effect), the Wannier exciton component can strongly interact with phonons. The combination of these two components will enhance the formation of phonoritons. Because hybrid excitons can be pre-designed, by varying the Wannier-Mott and Frenkel components, the room-temperature PMOSE will be numerically optimised aiming to minimise operating optical intensity.

The unique properties of the hybrid system will allow tuning the system to get the most preferable outcomes. One of the key points is to study the interaction of different components of the system with each other to get the condition to facilitate the observation of phonoriton and the phonon-mediated Stark effect.

Magnetic Transition-Metal-doped ZrO_2 Thin Films for Spintronic Applications

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We report about magnetic properties of transition-metal-doped ZrO_2 laser ablated thin films that are proven to be potential materials for spintronic applications. It is found that doping with a 3*d*-element can induce room temperature ferromagnetism in ZrO_2 semiconductor. Films of Fe/Co/Ni-doped ZrO_2 have shown nice magnetic domain structures that could be evidenced by magnetic force microscopy. Density functional theory simulations are in accord with experimental results, indicating that Mn- and Ni-doped ZrO_2 thin films have magnetic moments which are much larger than that of Fe- or Co-doped ZrO_2 thin films. Additionally, our calculations confirm that Mn- and Ni-doped ZrO_2 show a ferromagnetic ground state while Co- and Fe-doped ZrO_2 seem to favor an antiferromagnetic ground state. More importantly, it has been shown from our experiments that Mn- doped ZrO_2 thin films deposited on $LaAlO_3$ and YSZ substrates result in films with different types of structures then as consequence, different magnetic behaviors. One can conclude that the film thickness, as well as the interface between ZrO_2 semiconductor and insulating substrates, would play crucial roles in creating defects in this family of semiconductors. This finding can give precise guides for material search for suitable devices.

Electronic structure of novel two-dimensional materials

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Artificial two-dimensional (2D) materials, such as graphene or single-layer transition metal dichalcogenides, have electronic properties that are drastically different from those of their parent compounds. Moreover, these properties do not only depend on the 2D materials as such but also to their environment, for example on the substrate they are placed on. For instance, merely changing the dielectric properties of the substrate can strongly modify the band gap size of a 2D semiconductor.

Here we explore novel 2D materials such as single layers of MoS_2, WS_2 and TaS_2 by scanning tunnelling microscopy and (time-resolved) angle-resolved photoemission spectroscopy. The layers are grown epitaxially on Au(111), Ag(111) and graphene. For the semiconducting materials (MoS_2, WS_2), the Coulomb interaction in the layer can be controlled by the presence of the substrate or by excited carriers in the material as such, leading to a strong band gap renormalization. It is even possible achieve a semiconductor to metal transition in the materials, merely by the right choice of substrate.

1D Atomic Wires at Surfaces: Ultrafast non-Equilibrium Structural Dynamics in the Si(111)-In (8x2)<>(4x1) System at the Quantum Limit

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The Indium induced (4×1) reconstruction on Si(111) is a famous prototype for 1D atomic wires at surfaces. Indium atoms form parallel zigzag chains with anisotropic metallic conductivity. At 130 K a metal-insulator transition to the (8×2) ground state takes place. A Peierls-like distortion causes periodicity doubling, opening of a bandgap, and formation of a CDW. A robust hysteresis of 10 K width during temperature cycling proves that this phase transition is first-order [1]. The non-equilibrium structural dynamics of the (8×2) is studied by ultra-fast electron diffraction [2,3]. We use a pulsed electron gun in a RHEED geometry with a femtosecond-laser system in a pump probe setup. A tilted pulse front scheme [4] improves the temporal resolution to less than 350 fs. Upon photo excitation the (8×2) ground state is driven in 350 fs to the (4×1) excited state as observed through the transient RHEED spot intensity. The transition is described in an accelerated displacive excitation scenario which relies on transient changes in the potential energy surface. The population of specific long living electronic states facilitates the structural transition as they directly couple to the characteristic soft phonon modes. The strong coupling between substrate and adsorbate is responsible for the sub-picosecond structural response by dephasing and damping the characteristic phonons in 1/4th of their oscillation period – the transition proceeds in the regime of critical damping. Transient heating of the In atoms from 30 to 80 K occurs delayed on a time scale of 2.2 ps. Thus the phase transition is driven by electronic entropy and not thermally [4]. Cooling of the In layer to the substrate occurs on a time scale of 20 ps. An energy barrier for the atoms collective motion from the (4x1) state to the (8x2) state hinders the immediate recovery of the ground state: the In layer remains for nanoseconds in a super cooled metastable (4×1) state, which is not accessible under equilibrium conditions. The relaxation into the (8×2) ground state happens through the nucleation of the (8×2) at pre-existing adsorbates [5,6] which trigger a 1-dim. Recrystallization front propagating with 100 m/s as determined from a transient spot profile analysis of the (8×2) spots.

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Time-resolved spectroscopy of electron transfer processes at metal/organic interfaces

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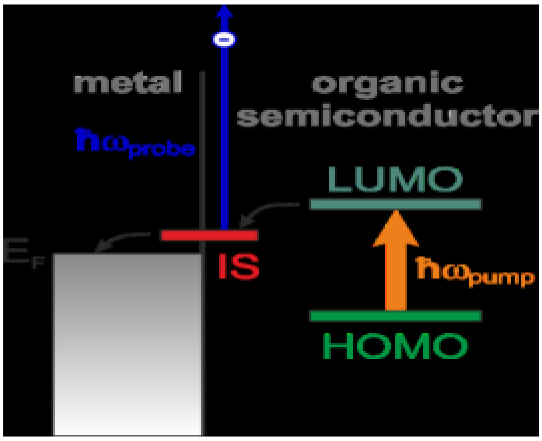
Interfaces between ordered organic thin films on single-crystal metals constitute well-defined model systems for electrical contacts of organic semiconductor devices. In this talk I will show that time-resolved two-photon photoemission (2PPE), a method that combines femtosecond pump-probe techniques with photoelectron spectroscopy, can provide detailed microscopic information about electron transfer and electron decay processes at such interfaces. Specific emphasis will be on the role of interface-specific electronic sates located between the Fermi level of the metal and the molecular LUMO.

Experiments with organic bilayer systems, such as CuPc/PTCDA/Ag(111) or PCTDA/TiOPc/Ag(111), unambiguously show that the normally unoccupied interface states (IS) can be optically excited from the metal side as well as from the LUMO of the second and even third organic monolayer. Transfer times of electrons form the LUMO into the IS and from the IS to the metal, determined directly in the time domain, range from 20 to 100 fs. These values indicate that the IS wave function has good overlap with both, the delocalized electron system of the metal and the relevant molecular orbitals. The IS is thus able to mediate the charge transfer between the metal and the organic semiconductor. The results show that not only the molecular level alignment at the interface, but also the properties of interface-specific electronic states play an important role for the efficiency of the charge transfer.



Work performed in the framework of the Collaborative Research Center “Structure and Dynamics of Internal Interfaces” (SFB 1083).

Excitations driven by femtosecond laser pulses in complex materials: Challenges and opportunities

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By now it is well know that optical excitation can change states of condensed matter and that the analysis of such excited states in the time domain provide insight into the nature of excited states including their characteristic timescales and their coupling to the environment. Also novel states which exist exclusively under the excited, non-equilibrium conditions may form. What is less well understood is in which limits simple heat bath models that are based on heat flow between spin, electron and lattice subsystems hold or fail. In this talk three examples (*i*-*iii*) are discussed. They highlight a variety of opportunities which become available by the specific excitation and the obtained non-equilibrium states. They build on non-thermalized quasiparticle distributions, non-equilibrium potential surfaces, and transient currents. (*i*) In cuprates we have identified a novel signature of electron-boson coupling using trARPES by a ten time increase of the quasiparticle relaxation time across a boson energy of 75 meV. This observation is indicative for a non-thermalized electron distribution due to coupling to one specific boson. [1] (*ii*) In the charge density wave compound RTe3 (R=Tb, Dy, Ho) the electronic gap function $\Delta(\mathbf{k})$ persists after intense optical excitation. A detailed analysis of trARPES data shows that $\Delta(\mathbf{k})$ is shifted in momentum space such that we conclude on a transiently enhanced Fermi surface nesting, which opens opportunities for steering broken symmetry ground states of matter under non-equilibrium conditions. [2] (*iii*) Quasi ballistic spin currents generated by femtosecond laser pulses in the Fe polarizer of Fe/Au/Fe/MgO(001) heterostructures interact with the Fe collector magnetization, which we probe by the time-resolved magneto-optical Kerr effect. Due to spin transfer torque a spectrum of spin wave excitations which is characteristic for the spin current pulses and the interaction at the ferromagnet's interface is generated. Analysing the spin wave spectrum we estimate a characteristic length scale of the spin transfer torque of 2 nm. [3] These examples suggest a wide variety of opportunities to manipulate, adapt and control excitations, material properties, and the dynamic response of complex materials after intense external optical stimuli.

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Ultrafast Electronic Structure Changes during Photoinduced Phase Transitions: The Dynamics of the In/Si(111) (8x2) ↔ (4x1) Transition

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We employ time- and angle-resolved photoemission spectroscopy (trARPES) to obtain a direct momentum-resolved view of the transient electronic structure during photoinduced transitions in charge density wave (CDW) systems. For the model CDW systems of the Tri-Telluride (RTe3) compounds we can directly map the dynamics of opening and closing of the CDW gap by trARPES and identify at least two Peierls-like amplitude modes [1]. Furthermore, we have developed a high-harmonic-driven XUV photoemission at 500 kHz repetition rate which provides complete access to the Brillouin zone in trARPES studies [2].

We investigate the ultrafast photoinduced insulator-to-metal transition of quasi-1D metal nanowires on In/Si(111) by trARPES. Starting from the insulating (8x2) phase we follow the gradual evolution of the electronic structure into the (4x1) phase on a femtosecond time scale. The gap at the (8x2) Brillouin zone center is observed to close already after 200 fs, while the states at the zone boundary shift from above to below the Fermi level within 500 fs. Moreover, the structural transition to the (4x1) phase, as manifested by the splitting of the m2-m3 bands, is completed after 700 fs. These data provide detailed insights into the transient population and evolution of the electronic structure which governs the forces acting during the photo-induced structural transition

In our trARPES study we also observe a coherent phonon mode at 2.4 THz (~80 cm-1), but no coherent modulation by the amplitude mode(s) as in the RTe3 [1]. The absence of a coherent excited amplitude mode together with the observed ultrafast electronic structure changes suggests a more complex scenario than a "standard" Peierls mechanism including rapid acceleration of surface atoms and fast energy exchange between In/Si surface modes. This is discussed in the context of recent time-resolved electron diffraction results and *ab-initio* molecular dynamics calculations [3,4].

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Ultrafast Low-Energy Electron Diffraction Enabled by Nanoscale Photoemitters

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Novel methods in ultrafast electron microscopy [1], diffraction and spectroscopy promise unprecedented insights into the dynamics of structural, electronic and magnetic processes on the nanoscale. A key to the realization of such technologies is the generation of high-quality beams of ultrashort electron pulses.

This talk will present the development and application of ultrafast imaging and spectroscopy based on localized electron sources, with a focus on Ultrafast Low-Energy Electron Diffraction (ULEED) [2,3]. Initially developed in a transmission geometry for monolayer and bilayer films [2], ULEED now allows for the study of structural dynamics from surfaces in backscattering diffraction [3]. Using this technique, we investigate the transformation between charge-density wave (CDW) phases at the surface of the transition metal dichalcogenide 1T-TaS_2. Harnessing the high transverse coherence of the low-energy electron beam, we resolve the coarsening of a nascent incommensurate CDW phase, and identify the phase-ordering kinetics with the annihilation of topological defects in the charge order.

In the future, based on a continuing miniaturization of ultrafast electron guns [4], ULEED will enable the study of structural dynamics in a wide range of surface systems, including surface reconstructions and molecular adsorbates.

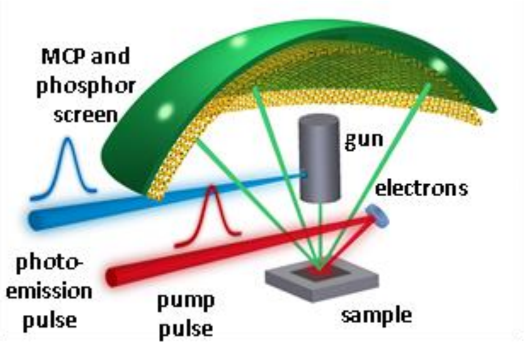

Fig. 1: Schematic of Ultrafast Low-Energy Electron Diffraction (ULEED)

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Ultrafast Dynamics of Surface Plasmon Polaritons

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Surface plasmon polaritons (SPPs) are collective oscillations of electrons at an interface between a noble metal surface and a dielectric material. Using grating couplers, structured by focused ion beam milling, it is possible to control the starting location of SPPs at the surface and to manipulate the shape of SPP phase-fronts on the nanoscale. Using photoemission electron microscopy (PEEM), the observation of SPPs is possible via a nonlinear photoemission process. In a normal-incidence experiment, where <15 fs short laser pulses impinge along the surface normal, a direct conceptual visualization of the SPP phase fronts is obtained [1]. Furthermore, a pump-probe experiment with sub-femtosecond temporal discretization provides for the recording of slow-motion movies of propagating SPPs [2]. In the presentation, the attainable time-resolved contrast and several examples of SPP propagation and interference will be discussed.

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Electron dynamics in the Rashba system BiTeI

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BiTeI is a layered semiconductor without inversion symmetry that shows a strong spin-orbit coupling leading to highly Rashba-split bands on the surface as well as in the bulk of the material. The polarity of this system creates differently charged surface regions depending on the surface termination. Such surface charges can be tuned by laser excitation, as has recently been observed on BiTe-based topological insulators [1]. This effect, known as surface photovoltage, occurs if the carrier lifetimes in a material are sufficiently long.

In time-resolved photoelectron spectroscopy using an angle-resolving time-of-flight spectrometer, we measured the population dynamics of excited carriers in Mn-doped BiTeI. Applying a 6.2-eV probe-pulse, we monitor the Rashba-split surface state and conduction band on the Te-terminated surface. Excitation with a 1.5-eV pump-pulse generates hot electrons with lifetimes of □ ~ 10 ps, which still follow a Fermi-liquid-like behavior. In contrast for equivalent hole excitations, we find a pronounced drop in the hole lifetimes shortly below E_F, which hints at the opening of a plasmon-emission channel as proposed in Ref. [2]. These strongly different electron and hole lifetimes, are generally expected to reduce the band bending at the positively charged Te-terminated surface. In line with this, we do indeed find a time-dependent shift in the chemical potential but without any change in the positions of conduction band and surface state, as would be expected for a surface photovoltage.

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Defects, doping and the CDW in $TiSe_2$

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1T-$TiSe_2$ is an unusual layered compound: it has not been conclusively established whether it is a small indirect gap semiconductor or a semi-metal; it has a charge density wave (CDW) that is stable below 200K; and it becomes superconducting under pressure, and following doping with Cu.

I will present the results of extensive experimental and theoretical investigations into defects in 1T-$TiSe_2$, focussing on scanning tunnelling microscopy (STM) and density functional theory (DFT) modelling. I will discuss the key native defects found (shown in Fig. 1): Se vacancies; I and O substituting for Se; and Ti self-interstitials[1]. I will discuss their identification, and their influence on the CDW[2].

I will then discuss two forms of doping and the effects on the CDW. Ti self-interstitials nucleate small domains of CDW[3] and can be found in two different locations relative to the CDW lattice[4]. The relative energies of these locations explain both the predominance of one over the other, and the CDW domains found. Cu also resides interstitially, and I will discuss our precise identification of its location as well as the stripe order that can be induced in the CDW, and the evidence for the origin of the CDW that comes from the visualisation of the Cu dopants.

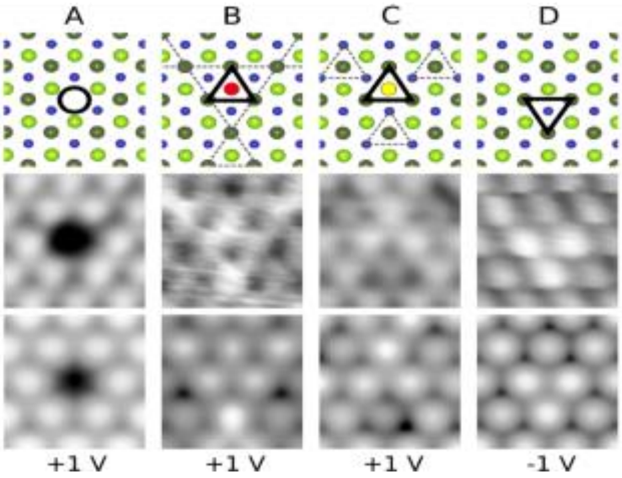

Figure 1. STM images (centre) (1.23×1.06 nm^2, I_t =200 pA, T =4.6 K), DFT simulated STM images (bottom) and schematic representation (top) for the four kinds of native defects in 1T –$TiSe_2$. (A) Missing Se_U atom; (B) Substitution of Se_D atom by an iodine atom; (C) Substitution of Se_D atom by an oxygen atom; (D) Ti self-interstitials[1].

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Thickness dependence of the charge density wave order parameter in thin exfoliated 1T-VSe_2

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We present a detailed scanning tunnelling microscopy (STM) study of the thickness and temperature dependences of the CDW order parameter in 1T-VSe_2. We show that mapping the real-space charge order over a broad and well-characterized thickness range, unique to STM, provides essential insight. We introduce a robust derivation of the local order parameter and transition temperature based on the real space charge modulation amplitude measured by STM (Fig.1a). Both quantities exhibit a striking non-monotonic thickness dependence (Fig.1b) that we explain in terms of a 3D to 2D dimensional crossover in the Fermi surface topology [1]. This finding highlights thickness as a true tuning parameter of the electronic ground state. Our results further reconcile seemingly contradicting thickness dependencies determined in independent transport studies [2,3].

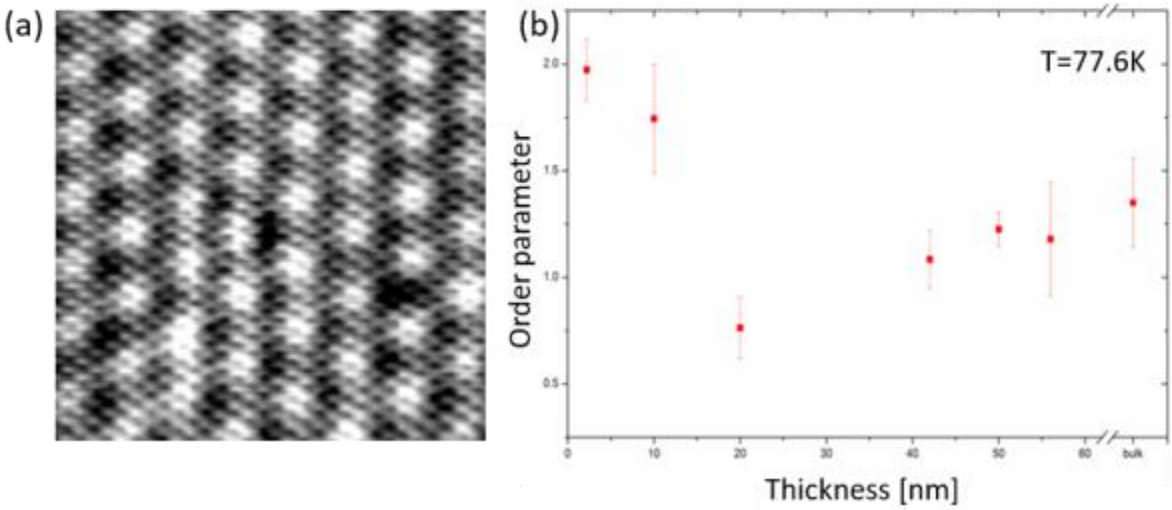

Fig.1 (a) 9x9 nm^2 high resolution STM micrograph at 77.6 K of the atomic lattice and CDW modulation on a VSe_2 nanoflake. (b) Thickness dependence of the CDW order parameter ψ calculated from the charge modulation imaged by STM. The error bars correspond to the dispersion of ψ across many different STM images at a given thickness.

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Dephasing in Strongly Anisotropic Black Phosphorus

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Black phosphorus (bP) is a direct band gap semiconductor, which, thanks to its layered structure, can be exfoliated down to the monolayer. It has attracted great interest for its various properties, among which anisotropic transport, optical, and thermoelectric properties have been recently observed and related to the puckered structure of the bP layers [1]. Here we present recent results on bP devices, in particular experimental observation of weak localization in a 65 nm-thick black phosphorus field effect transistor [2]. Weak localization (WL) is a quantum effect, related to coherent scattering at low temperatures. Using the Hikami-Larkin-Nagaoka model [3], the dephasing length Lφ (or inelastic scattering length) can be inferred from weak localization. Our study is performed for various gate voltages (Vg), in the hole-doped regime, at temperatures down to 250 mK (see Fig. 1). Lφ is found to increase with increasing hole density, attaining a maximum value of 55 nm at a hole density of approximately 1013cm-2. The temperature dependence of Lφ was also investigated. Above 1 K it decreases, with a weaker temperature dependence than T-1/2, the one expected for electron-electron interaction in two dimensions. Rather, the observed power law was found to be close to that observed previously in quasi-one-dimensional systems such as metallic nanowires and carbon nanotubes. We attribute this result to the puckered structure of bP which forms a strongly anisotropic medium for localization. Therefore, the anisotropic structure of black phosphorus plays a crucial role also for quantum interference effects such as WL.

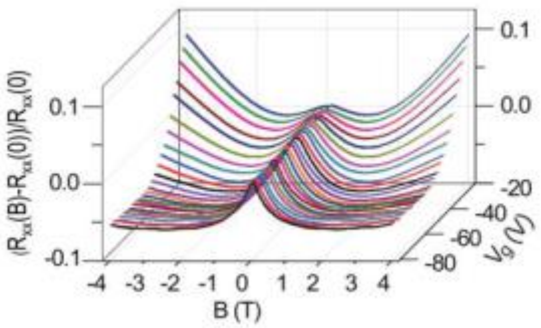

Fig. 1: Weak localization peak: plot of the normalized longitudinal resistance (Rxx(B)−Rxx(0))/Rxx(0) versus magnetic field B and back gate voltage Vg at T = 0.26 K.

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Germanene: graphene's little sister

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Recently, a few research groups have reported the growth of germanene, a new member of the graphene family [1]. Germanene is in many aspects very similar to graphene, but in contrast to the planar graphene lattice, the germanene honeycomb lattice is slightly buckled and composed of two vertically displaced sub-lattices. Frist principles total energy calculations have revealed that free-standing germanene is a two-dimensional Dirac fermion system, i.e. the electrons behave as massless relativistic particles that are described by the Dirac equation, i.e. the relativistic variant of the Schrödinger equation. We will give a brief update of the growth and electronic properties of germanene on Pt/Ge(110) nanocrystals [2,3]. Subsequently, we will show that large and continuous single germanene layers can be grown on molybdenum disulfide (MoS_2) [4]. The structural and electronic properties of the germanene layer are studied with scanning tunneling microscopy and spectroscopy. The lattice constant of the germanene layer is 3.8±0.1 Å, i.e. substantially larger than the lattice constant of MoS_2 (3.16 Å), and the interlayer distance between the germanene layer and the MoS_2 substrate is 3.2±0.2 Å, suggesting that we are dealing with a low-buckled germanene layer. The density of states of the germanene layer exhibits a V-shape, which is reminiscent for a two-dimensional Dirac system. The minimum of the density of states is located near the Fermi level.

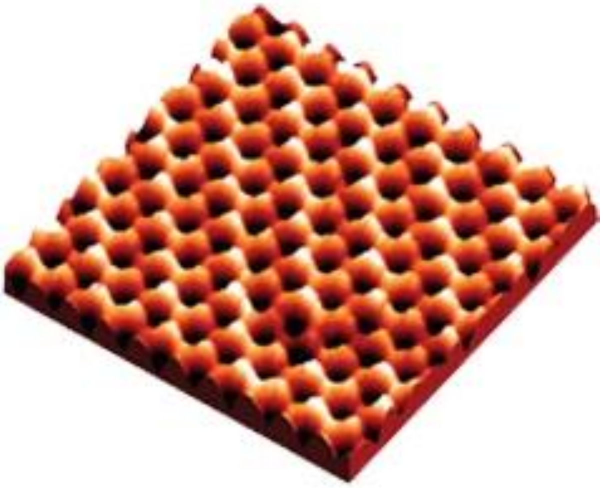

Figure caption Scanning tunneling microscopy image (4.5 nm by 4.5 nm) of buckled honeycomb lattice of germanene. Sample bias -0.5 V, tunnel current 0.2 nA.

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MoS2 enhanced T-phase stabilization and tunability through alloying and organic functionalization

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Recently two-dimensional layered materials based on transition metal dichalcogenides (TMD) have received a large amount of attention because of their peculiar and versatile physical properties [1]. Mono and few-layered TMDs are direct-gap semiconductors whose band gap energy, as well as carrier type (n- or p-) varies depending on the composition, structure and dimensionality of the system. In particular, monolayer MoS2 is known to exist in three polymorphs: 2H, 1T and 1T'. The former is thermodynamically stable and semiconducting (Egap=1.68 eV). The metallic 1T structure, on the contrary, was found to be metastable and undergo to a Peierls transition to the 1T' structure [2]. In the process a small energy gap (0.06 eV) is opened. In recent years, much effort has been made to stabilize T phases over 2H with the aim of gaining enhanced electrical performance, such as lower contact Schottky barriers, or better catalytic activity due to easier electron transfer. Although several techniques were proposed so far, such as alkali metals intercalation and straining, a proper control of
the transition is yet to be achieved. In this theoretical work, we propose two different routes for MoS2 T phases stabilization: alloying with an MX2 material for which the T phase is the thermodynamically stable one or functionalizing the monolayer with organic molecules. As for alloying realization, SnS2 is found to be the best candidate being known to privilege 1T structure over 2H (DE=0.87 eV). Indeed, results carried out by means of Density Functional Theory (DFT) and Cluster Expansion simulations show that, even for small amounts of Sn in MoS2, the T and T' phases formation energy is reduced making the switch between H and T easier. For low doping concentration, it is also reported that the MoS2 and SnS2 turn into metallic phases, opening up to the creation of metal-semiconductor junctions for PV cells [3].
DFT simulations were also employed to predict MoS2 functionalization with different organic
molecules, namely methyl groups and simple aromatic compounds. The proposed molecules are found to chemically bind to the T' phase of MoS2 monolayer and not to the H one. Our results not only show that these molecules can strongly modify the electronic properties of the MoS2 monolayer and effectively tune its absorption spectra, but also highlight that the stability of the two phases is inverted.

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Probing atomic and electronic structures of 2D electronic materials and their heterostructures

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The emerging atomic layer materials offer a remarkably wide range of building blocks of nanostructures ranging from metals (e.g. graphene), large gap insulators (BN), to semiconductors (transition metal dichalcogenides and black phosphorous). Key advantages of these van der Waals materials include a broad span of energy gaps, flexibility of stacking different types of materials to form heterostructures, tunability in material properties by doping and strain, and the relative ease of integration with other electronic and photonic devices. This talk will be focused on the usage of scanning tunneling microscopy and spectroscopy to probe the atomic and electronic structure of transition metal dichalcogenides (TMDs) and their heterostructures, including both vertical and lateral structure

I will first introduce a comprehensive form of scanning tunneling spectroscopy (STS) which allows us to probe not only the quasi-particle band gaps but also the critical point energy locations and their origins in the Brillouin Zone (BZ) can be revealed using this comprehensive form of STS. By using this new method, we unravel the systematic trend of the critical point energies for TMDs due to atomic orbital couplings, spin-orbital coupling and the interlayer coupling. By using the vertically stacked MoS2/WSe2, I will show how interlayer coupling can be used as a new designing parameter to create a lateral 2D electronic superlattices. I will then turn attention to MoS2/WSe2 lateral heterostructure where I will show a novel method to probe 2D strain tensor and how the strain changes the band profile as well as the band alignment at the interface.

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Interfaces between two atomically thin layers: structure and electronic properties

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Van der Waals (vdW) heterostructures have great potential in large-scale integration devices and new physics exploration. Experimental investigations allow flexible combinations of 2D crystals in interface fabrications. Theory, however, has limitations of supercell sizes and commensurability, translated into computational effort. To surmount these restrictions within first-principles investigations, we developed the coincidence lattice method, presenting a huge set of more than 700 interfaces with low simulation cost [1]. This allows systematic studies on bilayer heterojunctions and enables most interesting studies on vdW interfaces and devices. First, we investigate effects of stacking on transition metal dichalcogenides (TMDCs), showing that the electronic properties from the interface are affected by the structural conformation [1]. Then, we analyze effects of interlayer twist on a hBN/$MoSe_2$ heterointerface, concluding that hBN is a good substrate for preserving useful properties of $MoSe_2$, for its application in electronic and optoelectronic devices. We also show that interlayer twist angles play a significant role in the electronic properties of the substrate [2]. Finally, the tunability of band offsets via external factors is examined within bilayer interfaces of phosphorene and TMDCs. Consequences are derived from the contact, such as structural deformation, strong orbital hybridization, adjustable band offsets via electric field, and modulation of direct gaps by pressure [3]. These studies could help to find not only new physics within atomically thin interfaces, but to develop versatile electronic and optoelectronic devices as well.

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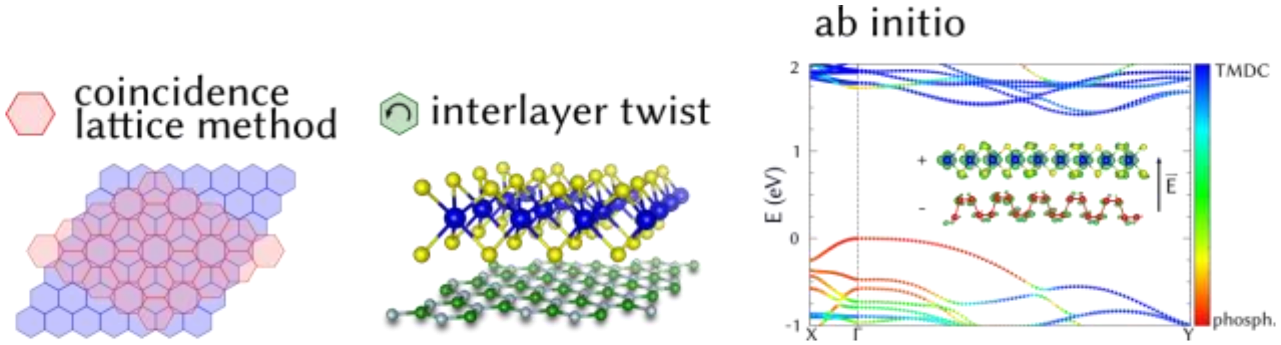

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Mechanistic Studies of Monolayer Doping of Semiconductor Surfaces for Ultra-shallow Junctions

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Efforts to continue reducing the dimensions of microelectronic components have driven efforts to develop processes to control materials synthesis, processes and architecture with atomic control for the next generation of transistors. As decreasing gate length dimensions become comparable to those of the depletion layers at the source and drain junctions, short-channel effects begin to dominate in emerging sub-10 nm devices. Consequently, there is an urgent need for precise and controllable methods for ultra-shallow doping of these junctions. Unfortunately, conventional methods of semiconductor doping that employ plasma treatments or ion implantation and annealing are incapable of producing abrupt, uniform doping profiles for length scales <10 nm with minimal surface damage. One promising new approach that has emerged to circumvent the aforementioned issues is monolayer doping (MLD). In the MLD process, a semiconductor surface is first functionalized with a single monolayer of a molecule containing the dopant of interest. The functionalized surface is then typically capped with thin inert overlayer (typically an oxide) to prevent evaporation, which is removed via acid etching after thermal processing. Finally, the substrate is subjected to a high-temperature annealing step to drive the dopants into the bulk. This novel approach has recently been demonstrated using self-assembled monolayers (SAMs) containing both p- and n-type dopants for MLD of silicon (Ho et. al., Nat. Mat., 7 (2008) 62-67) as well as various III-V compound semiconductors (Ho et. al, App. Phys. Lett. 95 (2009) 072108 and D'Costa et. al., App. Phys Lett. 104 (2014) 232102), and has been shown to result in high dopant densities with extremely shallow profiles. While these initial results have demonstrated the potential of the process, several issues remain such as the incorporation of carbon and surface composition inhomogeneities resulting from the SAM decomposition. Moreover, many fundamental aspects of the process remain unanswered and must be addressed for MLD to become viable for high-volume manufacturing. In particular, little is known about the fundamental surface chemistry and adlayer bonding configurations at each stage of the doping process, the role of native surface oxides, and the need for deposition of capping layers.

In this work, we describe a novel approach, based on conventional surface science, which does not require a capping oxide layer. We derive mechanistic information of MLD of Si and GaAs through a combination of *in situ* x-ray photoemission spectroscopy (XPS), low energy ion scattering (LEIS) and infrared (IR) spectroscopy, by examining the dopant/substrate interface as a function of thermal treatment. We find that the absence of a capping oxide layer allows the release of the hydrocarbon chain of the SAM layer prior to incorporation of the dopant atom into the semiconductor substrate. There is direct spectroscopic and electrical evidence that the dopant atom diffuses into the substrate, while the oxygen atoms remain at the surface. Broadband IR absorption measurements make it possible to quantify the density of activated dopant atoms in the near surface region. Using this particular example, this talk will highlight the importance of combining several surface science techniques to derive mechanistic information of technologically important structures.

Au Nanoantenna Arrays for Surface-enhanced IR Absorption

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Noble metal nanoantennas support localized surface plasmon resonances (LSPRs) 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 NCs. Here we present the results of an IR investigation of linear and H-type Au nanoantennas providing LSPR resonances at energies located in the mid- and far-IR spectral region making possible SEIRA by organic and inorganic nanostructures deposited on arrays of such nanoantennas. As a rule, only dipole active odd LSPR modes are excited at normal incidence in IR spectra of linear nanoantennas or nanorods. Here, we report that the activation of the even LSPR modes is possible in IR spectra of linear nanoantennas fabricated on a Si substrate measured under off- normal incidence of the light. With increasing angle of the incident light beam, the even LSPR modes become more prominent and LSPR modes reveal slight frequency shifts. The activation of even LSPR modes under off-normal incidence is explained by the lowering symmetry of linear nanoantennas fabricated on a Si substrate. All observations are confirmed by 3D electrodynamic simulations of nanoantennas. SEIRA by optical phonons in QDs as well as by organic ultra-thin (in nanometer range) films deposited on the nanoantenna arrays are discussed. 3D electrodynamic simulations were also used to calculate structural parameters of nanoantennas with different design providing the maximal SEIRA enhancement at the phonon energy in NCs. SEIRA spectra of the nanoantenna arrays with deposited monolayers of semiconductor NCs reveal distinct surface optical (SO) modes of the NCs [1]. The changes of the SO phonon mode intensities in SEIRA spectra of the nanoantenna arrays with the varied structural parameters quantitatively coincide with the changes of the magnitude of the averaged electric field intensity predicted from full-wave simulations. This work was supported by Russian Science Foundation (project 14-12-01037).

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Atomic structure and electronic properties of the 2D Tl-based compounds with √3×√3 periodicity on the Si(111) surface

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The Rashba spin splitting [1] in the two-dimensional electron gas systems on semiconductors is considered to be the key concept for many promising spintronics applications. Recently we found a number of the dense two-dimensional one-atom layer reconstructions on Si(111) surface with spin-split metallic bands [2]. One of these reconstructions made of one monolayer of Tl and one-third monolayer of Pb with √3×√3 periodicity was found to exhibit a giant Rashba-type spin splitting of metallic surface-state bands together with two-dimensional superconducting properties [3].

Our investigations revealed that the same type of the reconstruction with the same √3×√3 periodicity, composition and structure can be realized not only for 1 ML of Tl and 1/3 ML of Pb (Group IV element) but also for 1 ML of Tl and 1/3 ML of second adsorbate: Group I (Rb), Group V (Bi, Sb) and Group VI (Se, Te) elements. Our results indicate that the atomic arrangement of all compound layers is basically the same. They are composed of honeycomb-chained trimers of Tl atoms with Group IV, V and VI elements atoms occupying the T_1 sites in the center of each honeycomb unit while Group I element occupying the H_3 site. All of these two-dimensional compounds demonstrate spin split bands while their metallic properties changes dramatically if the second adsorbate is changed. Compound formed by Tl and Group IV element is metallic with two metallic bands, compounds formed by Tl Group V (Bi, Sb) and Group I (Rb) elements are also metallic with only one metallic band, while compounds formed by Tl and Group VI (Se, Te) elements are semiconducting.

The work was supported by the Russian Science Foundation (Grant 14-12-00479).

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Spin Dynamics of Individual Magnetic Impurities at the Surface of a Semiconductor

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Deposition and embedding at atomically-precise locations of individual magnetic impurities into semiconductor surfaces has been demonstrated with a variety of dopants, including especially transition-metal ions into III-V semiconductors[1]. Predictions[2], experimentally confirmed[3-5] have indicated how the magnetic dopants respond to local strain fields and the surface, but the resulting quenching of the magnetic moment through low symmetry and the spin-orbit interaction has made static measurements of magnetic properties very challenging[6].

Nevertheless it is possible to predict the expected results for dynamic measurements of magnetic properties and spin dynamics using electrical contacts such as are available using the scanning tunneling microscope. The focus here will be on pairs of magnetic impurities, that interact via the exchange or dipolar interactions[7]. Spin dynamics can be directly viewed through inelastic tunneling spectroscopy, or through low-field magnetoresistance measurements of magnetic dopant pairs.

This work was supported by the grant DE-SC0016447, funded by the U. S. Department of Energy, Office of Science.

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Quantum states of atomic defect nanostructures in silicon

Steven R. Schofield

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The quantum states formed by atomic point defects in semiconductors are of renewed current interest because these systems hold the potential to become the active components of nanoscale electronic devices with a range of exciting applications including quantum information processing. It is therefore critical that we develop a detailed knowledge of the nature of these states and develop methods for controlling their interactions. Scanning tunnelling microscopy and spectroscopy (STM/STS) provide the unique ability to resolve in real-space, and as a function of energy, the quantum states of individual defects, and to observe the changes as these states are coupled together or otherwise influenced by their local environment. In this talk I will present recent work exploring atomic-scale defects in silicon and their interactions using low temperature STM/STS. This will include a discussion of substitutional dopant states and surface deep-centre defects on Si(001) and Si(111). I will show that quantum interference, observable by STM/STS, arises between coupled defects for a range of defect types using both model calculations and first principles density functional theory calculations to support our interpretation.

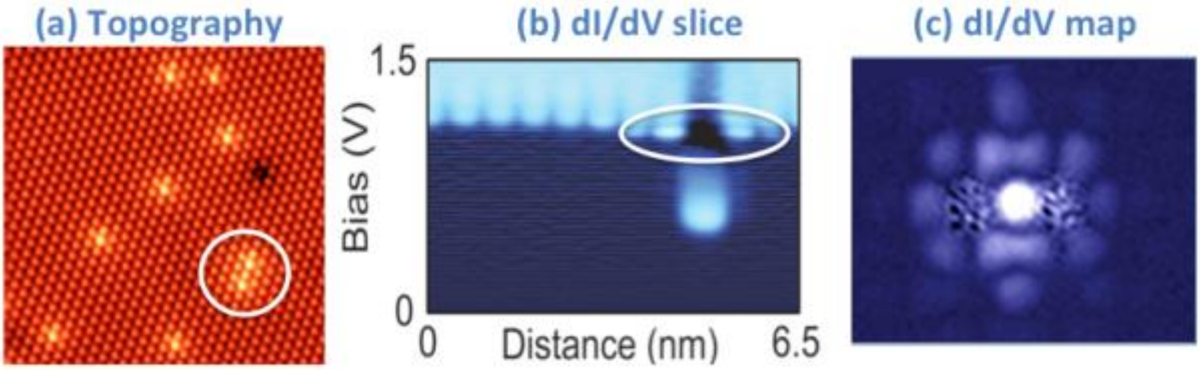

Figure 1: STM image and spectroscopy data for substitutional silicon defects in the B-terminated Si(111) surface. (a) Topography showing a large area image where a range of individual defects can be seen and one defect pair in the lower right. (b) Differential conductance slice through a single defect showing the defect excited state split off from the bottom of the conduction band. (c) Spatial map of differential conductance across a defect nanostructure exhibiting quantum interference.

Si(001)-AsH_3 : Arsine as Precursor to STM Patterned 2D Arsenic in Silicon

Taylor J.Z. Stock[1], Oliver Warschkow[2], Emily V.S. Hofmann[1], Steven R. Schofield[1], Neil J. Curson[1]

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[2] *Centre for Quantum Computation and Communication Technology, School of Physics, University of Sydney, Sydney NSW 2006, Australia*

STM hydrogen desorption lithography has been developed and utilized to great effect, resulting in device fabrication with atomically precise 2D patterning of phosphorous atoms in silicon. Expanding this technique to include atomically precise 2D patterning of two unique species of donor impurity atoms could provide new possibilities for device structure and function. For example, this could lead to the realization of optically driven silicon-based quantum gates, as proposed by Stoneham, Fisher, and Greenland.[1] Working towards this goal of STM lithographic fabrication with two species of donor impurities, we have used STM and DFT to examine the adsorption and dissociation of AsH_3 on Si(001), from low coverage to saturation, and from room temperature to 500 °C. The behaviour of this system is compared to the well-studied Si(001)-PH_3 system (precursor to the 2D patterning of phosphorous in silicon). While these chemically similar molecules may be expected to exhibit similar interaction with the Si(001) surface, we find that the dissociation of AsH_3 follows a pathway different from that previously determined for PH_3. This difference is attributed to kinetic limitations, and is used to explain the observed differences in concentration and structure of saturation coverages. In addition to adsorption behavior, we also discuss the incorporation, encapsulation, and electrical transport of As delta-layers, as well as the optimization of growth parameters required to utilize these delta-layers for atomic scale device fabrication.

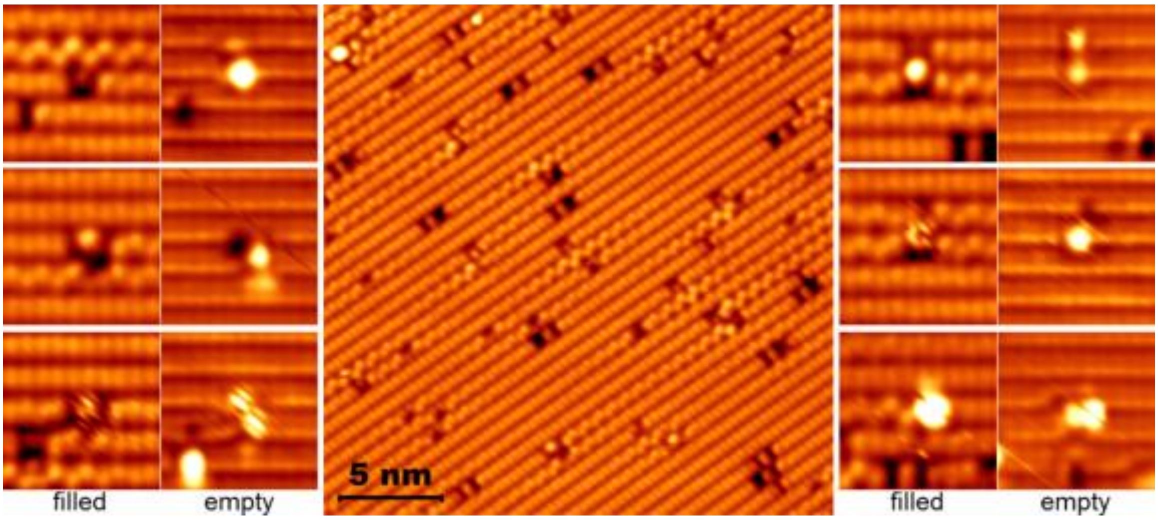

Figure 2: Filled state STM image of low coverage AsH_3 on Si(001) at room temperature showing multiple AsH_3 associated features. Filled and empty states images (3.84 nm) show details of the six unique features associated with AsH_3 and dissociation products.

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Computing in Silicon at the Atomic-Scale

Michelle Simmons

University of New South Wales, Australia

Down-scaling has been the leading paradigm of the semiconductor industry since the invention of the first transistor in 1947. However, miniaturization will soon reach the ultimate limit, set by the discreteness of matter, leading to intensified research in alternative approaches for creating logic devices. This talk will discuss the development of a radical new technology for creating atomic-scale devices which is opening a new frontier of research in electronics globally. We will introduce single atom transistors where we can measure both the charge and spin of individual dopants with unique capabilities in controlling the quantum world. To this end, we will discuss how we are now demonstrating atom by atom, the best way to build a quantum computer - a new type of computer that exploits the laws of physics at very small dimensions in order to provide a predicted exponential speed up in computational processing power.

Monday Tuesday Wednesday Thursday Friday Posters Author Index

STM-induced light emission: from molecular LED to subnanometric optical microscopy

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The electric current traversing the junction of a scanning tunneling microscope (STM) may generate a local emission of light. During the last years, we have used this method to study the intrinsic luminescence properties of individual molecules. This work has progressed in two directions. On one side we have used the ability of the STM to manipulate matter with atomic-scale precision to form single-molecule light emitting devices [1]. Composed by individual molecular wires suspended between the tip and the sample of the STM (see figure), these devices generate an emission of light whose color, intensity and bandwidth can be controlled with high precision [2,3]. On the other side, we used the intrinsic resolution of the STM to performed sub-molecularly resolved vibronic spectroscopy of molecules separated from a metallic surfaces by a thin insulating layers [4]. These results constitute an important step towards photonic measurements with atoms-scale resolution.

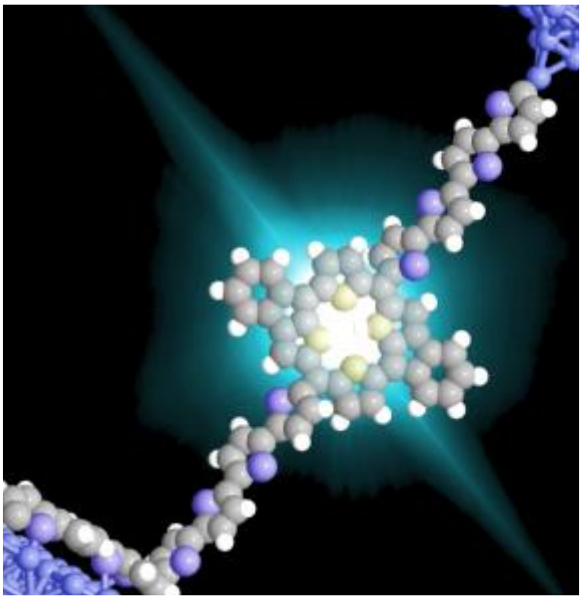

Figure: Artistic view of a single-molecule optoelectronic device operated with a scanning tunneling microscope

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Molecular self-assembled networks on boron doped silicon surface

Frank Palmino [1]

[1] *Institut FEMTO-ST, Université de Bourgogne Franche-Comté, CNRS, 15B Avenue des Montboucons, 25030 Besançon cedex, France*

Nowadays more than 90% of published results show molecules adsorbed onto metallic or HOPG surfaces. This is explained by the low reactivity between molecules and these surfaces which induce a molecular diffusion and the possibility to observe large and perfect self-assemblies. Nevertheless, there are a real economic and technological interests to develop molecular self-assembled layers onto semiconductors and in particular onto silicon surfaces. Actually, due to the existence of Si dangling bonds which induce a strong interaction between molecules and substrates, the formation of such molecular layers is still a real challenge. To circumvent this problem, we need atomically passivated Si surface. Here, an original unreactive silicon surface is presented: the high boron doped silicon √3x√3-SiB (111) reconstruction. Since 10 years, very amazing results have been obtained showing large and perfect molecular self-assemblies by deposition of home-made and specifically designed aromatic molecules on this silicon surface [See Fig. 3]. The morphology of each supramolecular network is explained by the competition between molecule-moleucle and molecule-surface interactions [1-4].

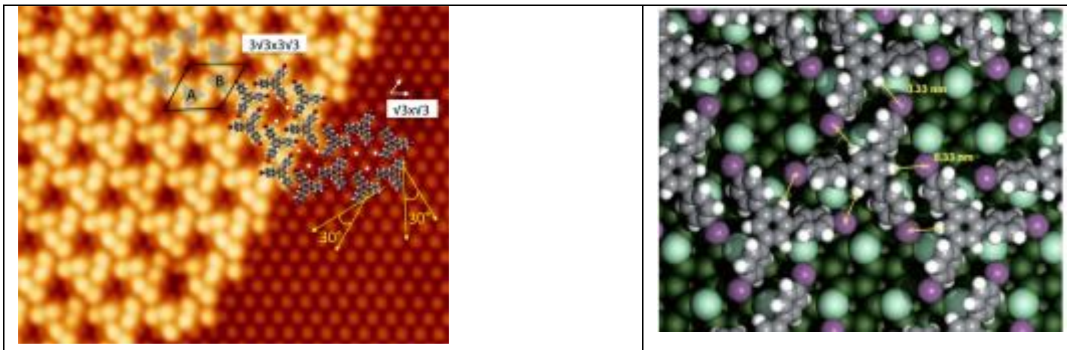

Fig. 3: Left: STM image of the molecular network (Vs=2.3 V, It=0.037 nA, 15x15 nm2).

Right: molecular model adsorbed onto Si(111)-B showing pi-stacking and halogen bonds interactions

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Interfaces of functional molecules with graphene and *h*-BN

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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. Bulk *h*-BN is an inert, electronically insulating and temperature-stable material. Thus, *h*-BN monolayers are widely used as templates with the potential to electronically decouple and spatially order atoms, molecules and nanostructures.

Here, I will first provide a comprehensive characterization of the *h*-BN/Cu(111) interface, including recent non-contact atomic force microscopy (nc-AFM) and X-ray standing wave (XSW) data. The main part of the talk will then focus on the interaction of functional molecules with *h*-BN/Cu(111) and graphene/Ag(111). E.g., tetrapyrroles 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, they are thus ideally suited as building blocks for versatile, surface-anchored nanostructures [1]. We apply low-temperature scanning tunnelling microscopy (STM), spectroscopy (STS) and nc-AFM in an ultra-high-vacuum setting to comprehensively characterize tailored molecule/sp^2 interfaces with sub-molecular resolution.

Specifically, I will address selected phenomena associated with the unique electronically super-structured *h*-BN/Cu(111) interface combined with tetrapyrroles and other functional molecules [2,3]. These include electronic decoupling, site-selective adsorption, site-selective gating, tip-gated charging, and intercalation. Additionally, I will present a dehydrogenative coupling reaction employed to fuse an archetypical tetrapyrrole to graphene edges and nanoribbons, where distinct bonding motifs are identified by nc-AFM (see Figure) [4]. These experiments provide access to new tetrapyrrole-based systems, metallo-supramolecular arrays and hybrid architectures with prospects for tunable functionalities, e.g., in sensing, heterogeneous catalysis or molecular electronics.

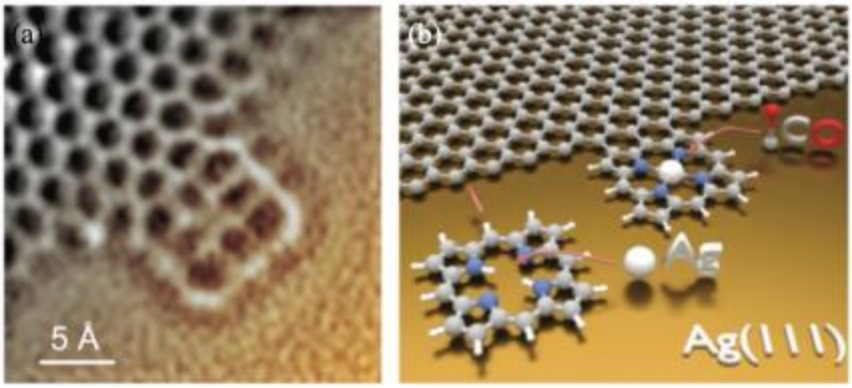

Figure: Tetrapyrrole fused covalently to a graphene edge: (a) nc-AFM image (b) scheme.

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Accommodation of the self-assembled perylene multilayer to Ag(110) surface morphology.

Kirill Bobrov, Nataliya Kalashnyk and Laurent Guillemot

Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris-Sud 11, F-91405 Orsay.

We present a room temperature STM study of perylene adsorption on Ag(110) in the monolayer to multilayer regime.

At the monolayer coverage regime perylene molecules form a quazi-liquid monolayer of epitaxial as well as self-assembling character. The monolayer accommodates the short-range thermal motion of the flat lying molecules instead of quenching it. The surface registry is provided by locking of one third molecules into specific adsorption sites of the (110) lattice. The monolayer structure and symmetry 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.

We found that increasing coverage preserves the thermodynamic balance while the molecules join the monolayer through π-π stacking, transforming it into a self-assembled epitaxial multilayer. We found that the thermodynamic balance bestows to the multilayer the unique quality to accommodate surface steps, naturally shaping any metal surface and usually preventing formation of defect-free epitaxial overlayers. We show that the perylene multilayer is able to spread over surface steps, to accommodate their thermal meander and to maintain the surface registry preserving its structure, integrity and single domain character. We analyze in details the multilayer structure which made possible the dynamic match-up of the multilayer and the underlying substrate.

The observed accommodation phenomenon opens perspectives to fabricate a defect-free single domain perylene overlayer on Ag(110) at an arbitrarily large scale.

Current-induced heating of carbene-based molecular junctions controlled by the interface

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Cukrovarnicka 10, Prague, Czech Republic

In this talk I will present our *first-principles* calculations of the current-induced heating and cooling dynamics of a series of molecular junctions based on N-heterocyclic carbenes on Au. I will show how in these systems the metal-molecule interface plays an essential role in determining not only the elastic transport properties of the junction [1] but also its current-induced heating dynamics under an applied bias. We study several interfaces where we consider different electrode terminations. With short blunt terminations, the molecule is strongly coupled and the cooling efficiency decreases monotonically as a function of the applied bias. This means that the temperature of the junction increases. With sharp chain-like terminations, the cooling ratio first decreases but then sharply increases at higher biases. This results in the effective cooling of molecular vibrations [2]. I will explain this behavior through a detailed analysis of the emission and absorption rates as a function of bias.

In the second part of the talk I will show how the presence of a NH_2 adsorbate in the proximity of the junction can influence its heating dynamics [3]. The molecule-adsorbate interaction induces changes in the molecular electronic structure which affect the cooling behaviour. We show that the NH_2 adsorbate acts as an external gating potential shifting the molecular states, and also causes a reduction of heating rates with bias. This sheds light on the role of adsorbates or contaminants adsorbed near the tunneling pathway.

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Adsorption kinetics of low density lipoproteins with langmuir monolayer

Ziad Khattari

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Abstract

The present work utilizes Langmuir monolayer technique to detect the adsorption kinetics of native low density lipoproteins and its oxidized form by lipid monolayer. We found that the low density lipoproteins and the oxidized low density lipoproteins are able to penetrate the LM up to pressure π=9.9 and 11.6 mN/m respectively. Also, the adsorption constants of both particles were found to depend strongly on the monolayer initial pressure. It is found that less compressed lipid monolayers could accommodate more native low density lipoproteins than the oxidized ones due their higher binding affinity toward monolayers. The probable α-helical regions along the apoproteinB-100 secondary structure and average hydrophobicity could explain partially their adsorption kinetics into lipid monolayers. This simplified 'in vitro' study of low density lipoproteins-monolayer interaction may serve as a step further to understand the mechanism and bioactivity of atherosclerotic process. Also, it may shed a light on the oxidized low density lipoproteins role on plaque formation in the innermost arterial wall in blood vessels.

Keywords

Langmuir monolayer; Atherosclerotic; LDL oxidation; Adsorption kinetics.

Quantum computing with rough multi-valley Si systems: electrically-driven spin and valley resonances and overcoming roughness

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[2] *Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies, UNSW Node, Sydney 2052, Australia*

The valley degree of freedom of Si has a strong effect on the operation of quantum-dot based qubits. For gate-defined quantum dots in the vicinity of Si interfaces the lowest-lying states belong to the two valleys perpendicular to the interface. These are connected by a valley-orbit coupling, which is a complex number with an amplitude and a phase, both of which are extremely sensitive to the interface roughness profile. In this talk I will demonstrate that in the presence of interface roughness steps: (i) a strong enhancement of electrically-driven spin resonance occurs as a result of the interplay of step roughness and intervalley spin-orbit coupling terms [1]; (ii) electrically-driven valley resonance and valley-state readout are feasible [2]; and (iii) the unwanted effect of interface roughness on the valley splitting and exchange between qubits can be mitigated by controlling the lateral gate voltage [3]. I will discuss the relationship between these findings and a series of recent experiments, and discuss their implications for Si-based quantum computing.

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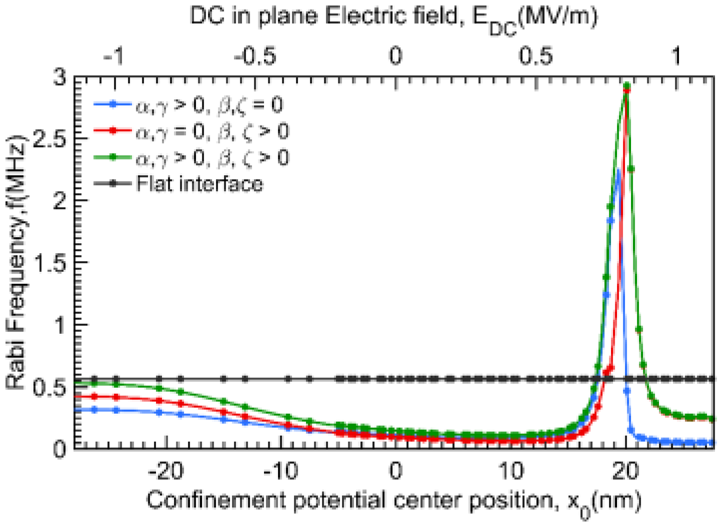

Spin-momentum-locked valleys in metal/semiconductor hybrid systems

Markus Donath

Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Spin-orbit interaction in combination with the broken inversion symmetry at surfaces induces spin-polarized electronic surface states with spin-momentum locking. The resulting spin landscapes are promising for spintronic applications. Metal/semiconductor hybrid systems such as heavy metal Tl overlayers on Si(111) or Ge(111) lie in the focus of current research because they provide metallic surface states with strong spin-orbit coupling on a semiconductor surface.

The Tl/Si(111)-(1x1) surface exhibits a surface-derived unoccupied state, which extends over the complete surface Brillouin zone [1]. It is known for its giant spin-orbit-induced spin splitting and unique symmetry-induced spin texture: a rotating spin pattern in momentum space along ΓK with completely out-of-plane spin-polarized valleys at the zone boundaries, oppositely oriented at the K and K’ points. Along ΓM, symmetry allows only pure in-plane spin polarization. The M point is encircled by this state. Its spin texture shows a peculiar twist, which reflects the C_{1h} symmetry of the M point. Doping of electrons by adding small amounts of extra Tl produces metallic valleys at K(K’). Spin-resolved inverse photoemission with a ROtatable Spin-polarized Electron source (ROSE) was used to reveal the complex spin texture of the unoccupied surface bands [2].

A comparative study on Tl/Ge(111) provides surprising results [3]: The spin splittings of the surface bands are much smaller than on Tl/Si(111) despite the stronger surface localization and the heavier substrate. Model calculations show that a remarkable interplay between spin-orbit coupling and hybridization is responsible for this unexpected result. The strength of the spin-orbit coupling alone, based on the atomic number of the respective elements, is not sufficient to estimate the spin splittings of spin-orbit-influenced surface states.

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Surface Attophysics

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Femtosecond and subfemtosecond time scales typically rule electron dynamics at surfaces. I will analyze briefly electron dynamics at surfaces and nanostructures with emphasis on surface attophysics, namely streaking experiments and spin dependence of charge transfer at adsorbates.

Spin-texture inversion in the giant Rashba semiconductor BiTeI

Hendrik Bentmann, Henriette Maaß, Friedrich Reinert[1]

[1] *Experimental Physics 7, University Würzburg, 97074 Würzburg*

Semiconductors with strong spin–orbit interaction as the underlying mechanism for the generation of spin-polarized electrons are showing potential for applications in spintronic devices. Unveiling the full spin texture in momentum space for such materials and its relation to the microscopic structure of the electronic wave functions is experimentally challenging and yet essential for exploiting spin–orbit effects for spin manipulation. Here we employ a state-of-the-art photoelectron momentum microscope with a multichannel spin filter to directly image the spin texture of the layered polar semiconductor BiTeI within the full two-dimensional momentum plane. Our experimental results, supported by relativistic *ab initio* calculations, demonstrate that the valence and conduction band electrons in BiTeI have spin textures of opposite chirality and of pronounced orbital dependence beyond the standard Rashba model, the latter giving rise to strong optical selection-rule effects on the photoelectron spin polarization.[1] These observations open avenues for spin-texture manipulation by atomic-layer and charge carrier control in polar semiconductors. We shall cross-compare our observations of selection-rule effects on the photoelectron spin polarization to related experiments on layered topological insulators.

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Oleg E. Tereshchenko, Konstantin A. Kokh, Evgueni V. Chulkov, Jürgen Kirschner & Friedrich Reinert,
Nature Communications **7**, 11621 (2016)

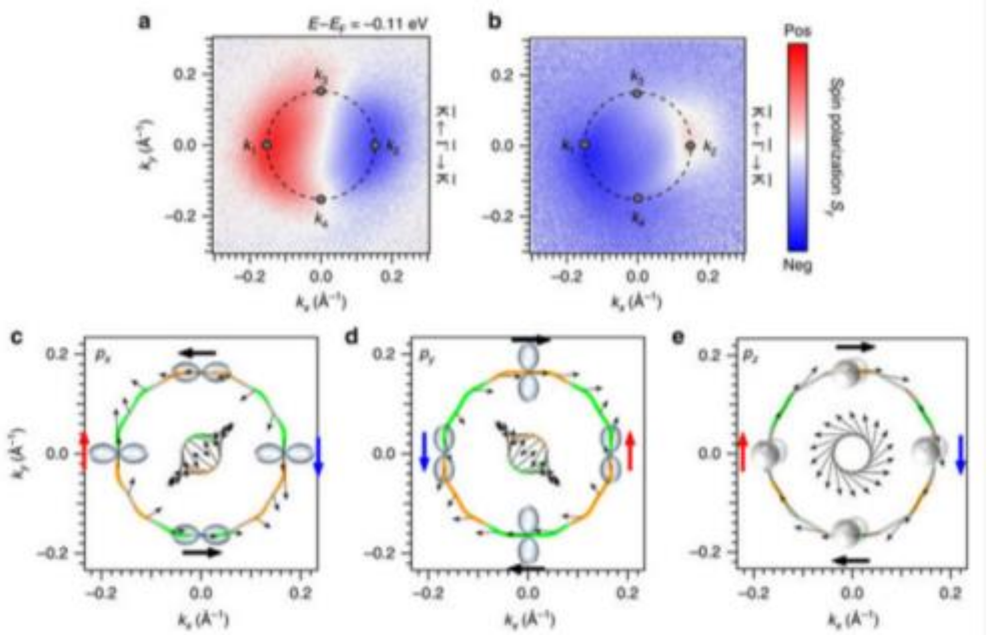

Figure 1: Spin-resolved ARPES data of spin-orbit split electronic states in the polar semiconductor BiTeI(0001) for (a) s-polarized and (b) p-polarized light. (c)-(e) First-principles calculation of the spin-polarization and the orbital character of the electronic states [1].

Polarization Doping and Work Function of Epitaxial Graphene on Silicon Carbide

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[1] *Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz, Germany*

[2] *Lehrstuhl für Laserphysik, FAU Erlangen-Nürnberg, Staudtstr. 1, 91058 Erlangen, Germany*

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, and $g_s = 2$ 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.

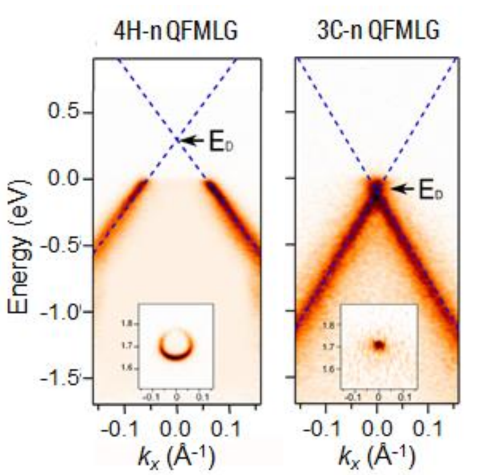

Fig. 1: π-bands of graphene on hydrogen-terminated, n-type 4H-SiC(0001) and 3C-SiC(111) probed by ARPES in the vicinity of the K-point of the hexagonal Brillouin zone. The position of the Dirac point E_D is marked.

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 [3]. 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.

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Graphene as a substrate: 2D layer van der Waals epitaxy and 1D nanowires

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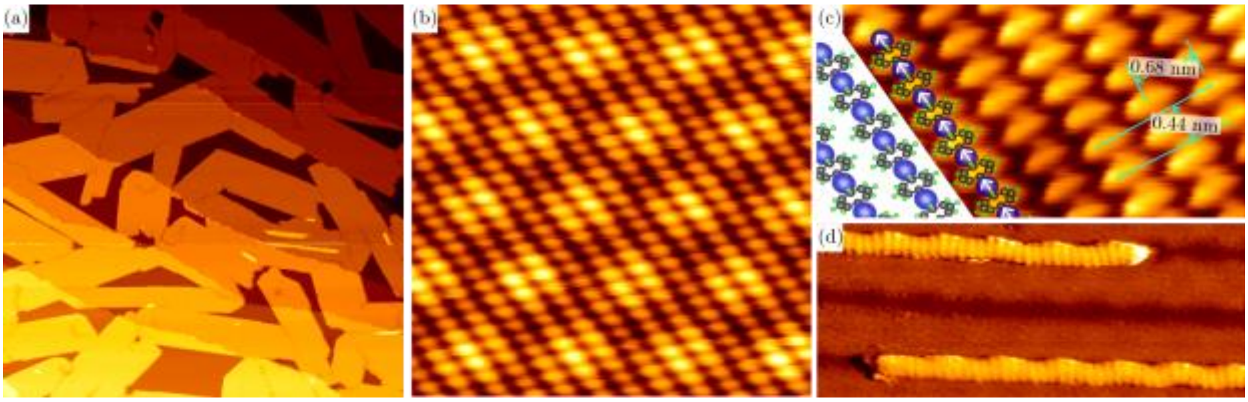
Graphene is a substrate of excellent structural quality and with electronic properties than can be tuned by doping. In the present talk two applications of graphene as a substrate will be highlighted.

First, graphene (Gr) enables oriented growth of transition metal dichalcogenide layers as well as textured growth of oxide thin films. This statement will be exemplified through results on growth and properties for the ferromagnetic semiconductor EuO grown on Gr. The excellent structural quality achieved enabled for the first time the observation of its magnetic surface state that has been predicted already in 2001.

Second, a new on-surface synthesis method is reported that enables the growth sandwich molecular nanowires. The synthesis is based on the use of Gr as an inert substrate and relies on the simultaneous deposition of metal atoms and organic ligands. Through the inert substrate, the molecule - metal atom reaction and the attachment of the reactants to existing wires are favored over mere adsorption to the support. Compared to a gas phase reaction, the encounter probability of the reactants with each other and already formed nanowires is enhanced. These nanowires are a new class of 1D magnetic entities, distinct from 0D single molecule magnets and 2D organo-metallic networks. Our synthesis method is exemplified for sandwich molecular wires consisting of Eu atoms and cyclooctatetraene (Cot) molecules. The resulting EuCot sandwich molecular nanowires are shown to be ferromagnetic semiconductors.

Contributions to this work by Lucas M. Arruda, Nicolae Atodiresei, Matthias Bernien, Andrew J. Britton, Carsten Busse, Fabian Craes, Daniel F. Förster, Felix Huttmann, Jürgen Klinkhammer, Stefan Kraus, Wolfgang Kuch, Hans P. Oepen, Katharina Ollefs, Fabian Nickel, Nico Rothenbach, Sven Runte, Nicolas Schleheck, Martin Schlipf, Stefan Schumacher, and Heiko Wende are gratefully acknowledged.



STM topographs of a submonolayer film of EuCot nanowires on graphene/Ir(111). (a) (330 nm)^2 overview of SMW islands covering the surface. (b) (10 nm)^2 Zoom displaying molecular resolution of the wire to which the Gr moiré with Ir(111) is superimposed as height modulation with 2.5 nm periodicity. (c) (5x2.5) nm^2 high resolution topograph partially overlaid with a structural model and a possible spin structure. (d) (22x9) nm^2 STM topograph of single, well separated SMWs grown on a nanopatterned substrate. From: F. Huttmann, N. Schleheck, N. Atodiresei T. Michely, submitted.

Spin-Polarized Four-Probe STM Study on Spin Transport of Topological Insulators

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Spin-polarized four-probe STM is developed by advancing two well-known STM-based techniques, spin-polarized STM and four-probe STM, to achieve spin-sensitive multi-probe characterization of thin films and nanostructures. Here we demonstrate its applications in detecting spin-chemical potential on pristine topological insulators surfaces in the UHV environment. By examining the potential difference between a ferromagnetic probe and a nonmagnetic probe as a function of the spatial separation of them, not only can we differentiate surface and bulk contributions to the conductivity, but also isolate the non-vanishing spin-dependent electrochemical potential from the Ohmic contribution for the first time. Moreover, the spin-sensitive probe method with nanometer scale soft contacts minimizes metal induced effects on the surface. The measured spin chemical potentials directly come from the 2D charge current. In this manner, we achieve a direct and quantitative measurement of the intrinsic spin-polarized transport associated with topological surface states. This method provides a direct measurement of spin current generation efficiency and opens a new avenue to access the intrinsic spin transport associated with pristine topological surface states.

Investigation on Metal-Graphene-Semiconductor (MGS) Interfaces

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The present paper deals with the metal-graphene and graphene-semiconductor (MGS) contacts aiming design and implementation of modern electronic devices for analog very high frequencies operations and higher power applications. This is due mainly to the higher electron mobility and power sustainability of graphene material. For metal-graphene MG contacts, MLG (multilayer graphene) are good candidate for Schottky diodes and MESFETs. In addition, the MGS structure can also be used for design of better photovoltaic cells [1].

Recently, graphene has been widely studied aiming a variety of devices and applications [2] that led to the emerging of Carbon electronics. Graphene electronic characteristics such very high electron mobility and thermal sustainability made of it a candidate for future electronic devices. However, understanding of the metal-graphene junction (MGJ) [3] is crucial for improving the transmission from metal to grapheme and vice versa [4]. This will reduce the MG contact resistance and lead to efficient FET devices. Moreover, getting thermal stability for the MG contacts can overcome the major concern in conventional MESFETs.

Graphene semiconductor contacts are being widely studied [5,6], as they are basics for designing Schottky barrier devices. The MGS semiconductor structure can lead to high performances devices and MEMS.

The present work is meant to study the transport properties in the MGS both MG and GS aspects aiming understanding and modeling of the transport at higher nobilities and under high temperatures.

To achieve the study, we have considered the band structure of the structure and explained the mechanisms of current conductions at higher mobility. The MG contact is studied based on a GFET and the GS junction based on a HEMT. Some other features are studied based on photoconduction and emission.

We concluded that, the MGS based devices can be of great help in designing new high power and higher frequencies devices and sensors.

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Few-layer graphene with self-aligned nanodomain boundaries on SiC/Si(001): Atomic structure, transport and magnetic properties

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Few-layer graphene exhibits exceptional properties that are of interest both for fundamental research and technological applications. The abilities to open energy gap and to make graphene magnetic are principal challenges in the fields of graphene-based electronic and spintronic applications. Nanostructured graphene with a large number of domain boundaries and ripples is one of the promising materials because the nanodomain edges can perfectly reflect electrons over a large range of energies [1] and host spin-polarized electronic states [2,3]. Additionally, transport gap opening and spin–orbit coupling can be induced by ripples at the graphene domain edges. In this report we discuss the atomic structure and electron transport properties of uniform nanostructured few-layer graphene with self-aligned boundaries synthesized on the technologically relevant SiC(001)/Si(001) wafers [4-6]. Our transport measurements demonstrate that fabrication of such nanodomain system leads to the transport gap opening at temperatures below 100 K [6]. Magnetic transport measurements reveal an unprecedented large positive magnetoresistance in parallel magnetic field with a strong temperature dependence [7]. According to the theoretical calculations performed for different domain edge structures, the transport and magnetic properties of graphene/SiC(001) are related to the localized states at the nanodomain boundaries. Our results show the feasibility of creating new electronic nanostructures using graphene on SiC/Si(001) wafers.

This work was partially supported by the Russian Academy of Sciences, Russian Foundation for Basic Research (grant № 17-02-01139, 17-02-01291), Beijing Institute of Technology Research Fund Program for Young Scholars, and Marie Curie IIF grant within the 7th EC Framework Programme.

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Modulation of electron-phonon coupling in one-dimensionally nanorippled graphene on a macrofacet of 6H-SiC

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Electron-phonon coupling plays various roles in solids such as inducing phase transitions and electron energy relaxation. In graphene, it is actually one of the dominant sources of the energy relaxation. Electron-phonon coupling can be detected by tunneling spectroscopy as an increase of the tunneling current at the absolute value of the sample-bias voltage corresponding to the phonon energy through an inelastic tunneling process.

Here, we report local electron-phonon coupling of a one-dimensionally nanorippled graphene on a SiC(0001) vicinal substrate. We have characterized local atomic and electronic structures of a periodically nanorippled graphene (3.4 nm period) prepared on a macrofacet of the 6H-SiC crystal using scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoelectron spectroscopy (ARPES). The rippled graphene was made by thermal decomposition of a vicinal 6H-SiC substrate. A typical image of the rippled graphene is shown in Fig. 1(a). Replica bands due to the periodic modulation of the graphene lattice are detected by the macroscopic ARPES measurements as in Fig. 1(b). We focused on the inelastic tunneling due to the out-of-plane phonon at the K points of graphene, which was clearly observed as a gap-like feature of 0.13 V wide around the zero-bias voltage in the dI/dV spectra. [1] The STM/STS results shown in Fig. 1(c) indicate the strength of electron-phonon coupling is periodically modified in accordance with the ripple structure. We propose that the carbon monolayer including graphene nanoribbons at the interface between the surface nanorippled graphene and the substrate SiC periodically modifies the electron-phonon coupling in the surface graphene.

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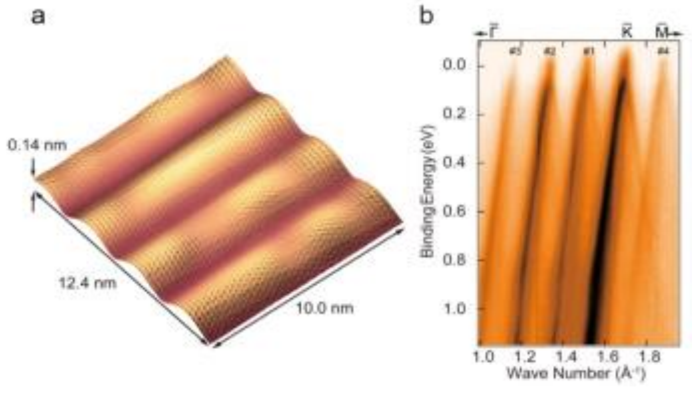

Figure 1 STM image (a) and ARPES results (b) of the nanorippled graphene on a macrofacet of the 6H-SiC.

Chiral Solitons in Atomic Wires: Toward Multi-digit Topological Computation

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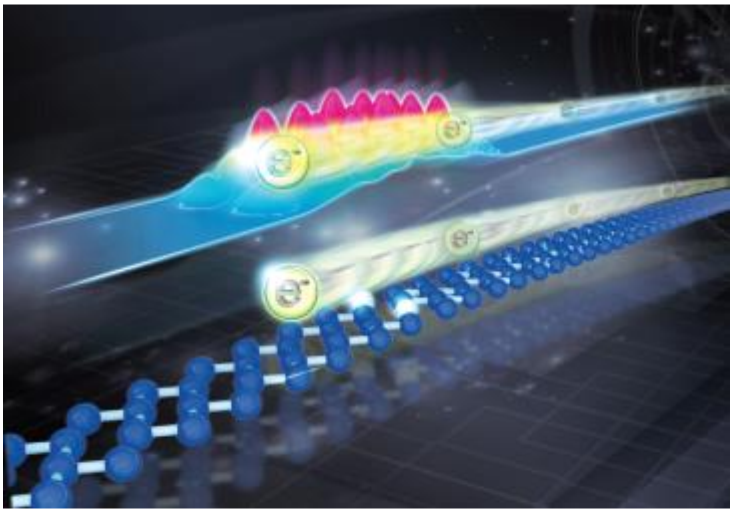

Storing and manipulating information in robust ways is of prime interest in various fields of science and technology. Using topologically protected local excitations, such robust informatics may be realized. In magnetic information processing, the recent interest is focused on topological excitations of spins such as skyrmions. In electronic systems, Majorana Fermions are expected to realize topological quantum computation. This talk reviews our recent approach to this issue, which deals with new types of solitons in electronic systems. We will discuss an one dimensional topological insulator, atomic wires in a charge density wave ground state [1, 2], and its soliton edge states [3, 4]. We recently identified individual electronic solitons in indium atomic wires on silicon surfaces [3]. Due to the wire's unique structure composed of double Peierls atomic chains, this system constitutes an unprecedented Z_4 topological system and its edge excitations correspond to solitons with chiral dimension [4]. These chiral solitons can store multi-level information, which is protected topologically. We further demonstrate the switchability or the algebraic structure of this multi-level information through the newly found soliton-soliton interaction [5], which indicates these information carriers operational. Thus, the possibility of multi-level, topologically protected, information processing is demonstrated for the first time.

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Band offsets and ordering in III-V nanowires determined by STM and STS

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Compound semiconductor nanowires (NWs) are promising building blocks for novel (opto)electronic and energy harvesting devices. Their efficiency depend critically on the (i) interfaces between different structural or compositional segments within III-V semiconductor NWs and (ii) on the ability to taylor new types of chemical ordering in ternary NW segments. Scanning tunneling microscopy (STM) and spectroscopy (STS) is an ideal tool for the high resolution analysis of both effects.

First, unfortunately the band gaps and band offsets at interfaces were thus far is mostly wrongly interpreted in literature: The commonly high step density at the sidewalls of III-V semiconductor NWs leads to extrinsic surface states pinning the Fermi energy within the fundamental band gap. Since the pinning level is different on every polytype and material composition, the relative band edge positions between different types of NW segments are extrinsically determined, but not by intrinsic band offsets. The extrinsic band offsets are much larger and likely have a stronger influence on the carrier transport than intrinsic band offsets. This problem is intrinsic to any surface sensitive characterization technique. Thus, we applied a new methodology to accurately determine band offsets between different NW segments by using a thin overgrown shell of a material with a wider band gap which assures that the Fermi level pinning of both segments is identical. Tunneling through the thin shell probes the band edge position of the underlying core materials under defined pinning conditions, providing the intrinsic band offsets. We illustrate the physical effects on interfaces of wurtzite/zincblende GaAs and GaAsSb/GaAs NWs.

Second, we reveal the existence of an unrecognized chemical ordering in ternary III-V materials. The lazarevicite short-range order, found in the shell of $InAs_{1-x}Sb_x$ nanowires, is driven by the strong Sb-Sb repulsion along [110] atomic chains during their incorporation on unreconstructed {110} sidewalls. Its spontaneous formation under group-III rich conditions of growth offers the prospect to broaden the limited classes of ordered structures occurring in III-V semiconductor alloys.

Clarifying the electronic structure of rare earth silicide nanowires on Si(001)

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Trivalent rare earth metals are well known for their formation of metallic hexagonal silicides with exceptionally low Schottky-barrier heights to *n*-type Si. Due to their anisotropic lattice match to the Si(001) surface, these silicides grow as self-organized nanowires, exhibiting widths of only few nanometers and lengths of several hundred nanometers. The general electronic structure of the nanowires is expected to be independent of the rare earth metal because of the uniformity of their atomic structures, which is verified by their similar appearance in scanning tunneling microscopy (STM). However, the appearance of the reported band structures of Dy and Er silicide nanowires was found to differ from the one observed for Gd silicide nanowires [1,2].

Here, angle-resolved photoemission spectroscopy (ARPES) was used to study the electronic structures of Y and Tb silicide nanowires in detail [3]. In contrast to prior studies, we obtained three-dimensional ARPES data (see Fig. 1). In this way, the assumed quasi-one-dimensional electronic structure is confirmed conclusively, since the Fermi contours are only slightly oscillating and do not form closed curves. This also agrees with the observation of a Peierls-like transition for Y silicide nanowires typical for quasi-one-dimensional metals [4]. Furthermore, the discrepancies in the appearances of the reported band structures are resolved by the observation of strong matrix element effects in our data. All bands described in the literature are observed for certain values of *k*y, and an additional band reaching the Fermi level is resolved.

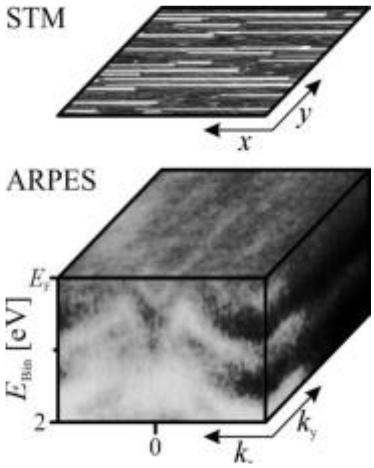

Figure 1 Real space and k-space data of Tb silicide nanowires.

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Strain induced quasi-one dimensional structure of rare earth silicides on Si substrates

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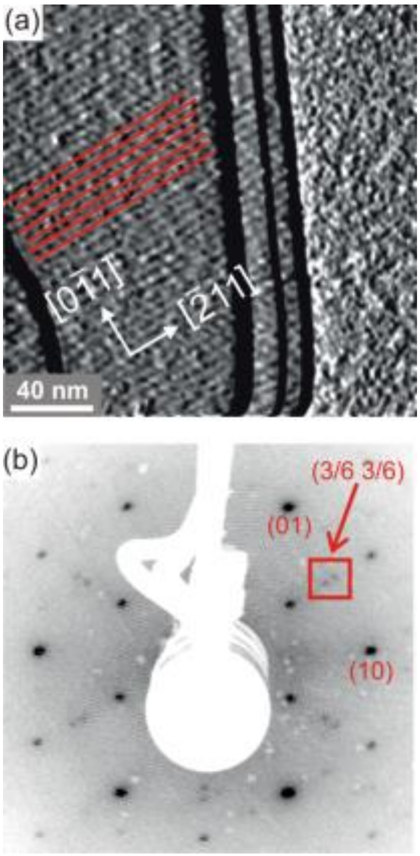
One dimensional (1D) systems have attracted a lot of attention since their physical properties are distinctively different from structures of higher dimensionality. Recently, a new class of quasi-1D systems based on rare earth silicides (RESi) has attracted attention since RESi monolayers form a large variety of different superstructures on Si substrates (cf. [1] for Si(111)). Some of these superstructures have large anisotropic quasi-1D structures. This effect has been attributed to strain induced effects due to different 'bulk' structures RESi and Si [2].

Here, we report on combined studies on quasi-1D structures by scanning tunneling microscopy STM), spot profile analysis of low-energy electron diffraction (SPA-LEED), and density functional theory (DFT) to shed light on the complexity of these structures. Depositing rare earth elements (Dy, Tb) at elevated temperature on Si(111), a $2\sqrt{3}\times\sqrt{3}$ superstructure is observed [3,4]. This structure is attributed to the formation of periodically arranged Si vacancies in different silicide layers. The complex structure of this superstructure with buckled surface layer, $\sqrt{3}\times\sqrt{3}$ superstructure in the first subsurface layer $2\sqrt{3}\times\sqrt{3}$ superstructure in the second subsurface layer can only be analyzed applying the different techniques used here. The anisotropic character of this structure is emphasized by the formation of periodically arranged domain boundaries. The width of the silicide domains formed in two domains is roughly two unit cells.



Si(111)-RESi$_2$-(2√3x33). (a) STM mircrograph showing quasi-1D structures. (b) LEED picture with split diffraction spots, e.g, (3/6,3/6) peak.

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Spin polarization of spin-orbit coupled states studied by laser-SARPES

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We have developed a laser-based spin- and angle-resolved photoelectron spectroscopy (laser-SARPES) apparatus at the Institute for Solid State Physics, The University of Tokyo [1]. Here Iwill present the design and performance of our laser-SARPES machine. I will also show the study of thespin-orbital entangled states of strongly spin-orbit-coupled (SOC) materials by laser-SARPES [2-4].

Design and performance of the spectrometer

In our system, the electrons are excited 6.994-eV photons, which correspond to the 6th harmonic of a Nd:YVO4 quasi-continuous wave laser. The photoelectrons are analyzed by a ScientaOmicron DA30L analyzer equipped with an electron deflector function. To analyze the spin polarization three-dimensionally, two very-low-energy-electron-diffraction (VLEED) type spin detectors are orthogonally placed each other. The combination of the high-performance spectrometer and the high-photon-flux laser achieves an energy resolution of 1.7 meV for SARPES.

Spin-orbital entangled states and spin polarization of photoelectrons

The strongly SOC materials such as topological insulators and Rashba systems are intensively studied not only because of fundamental interests but also technological directions. In a standard model of the spin texture of the SOC materials, the spin is locked to the momentum of an electron. However, recently, the spin-orbital entangled states were discovered in topological surface states. Here we show the spin-orbital texture of a Bi(111) surface state and draw a general description of the spin-orbital texture of the SOC systems in the mirror symmetry. Moreover, we establish a model of three-dimensional spin-rotation effect in photoemission process [4]. The laser-SARPES measurements were performed in a mirror plane of the Bi(111) surface. We observed the spin polarization only in the direction perpendicular to the mirror plane with *p*- and *s*-polarized lights. We also found the reversal of the spin polarization upon switching the light polarization from *p* to *s*. Thus, a spin-polarized branch consists of the linear combination of |ψeven,↑> and |ψodd,↓> states. On the other hand, even if the mirror symmetry governs the spin orientation in the initial states, rotating the electric-field vector of the incident linearly polarized light can break the mirror symmetry of the experimental geometry, which leads to the three-dimensional spin rotation in photoexcited states. This is produced by the spin-dependent quantum interference of the wavefunctions, resulting from simultaneous excitation of the |ψeven,↑> and |ψodd,↓> states.

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Weak spin injection in epitaxial MnGa/GaN

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The efficient realization of spin-injection and spin-detection is a prerequisite for many new device concepts in the field of semiconductor spintronics. However the conductivity mismatch in hybrid metal/semiconductor systems generally limits the spin-injection efficiency in the diffusive transport regime. Still, tunnel barriers might be employed in order to overcome this problem. In this paper, an experimental study of spin injection through reverse biased MnGa/GaN Schottky diodes is presented. Ferromagnetic MnGa(111) layers with high crystal quality were grown on GaN(0001) by molecular beam epitaxy. The doping of the structure was optimized to achieve single step tunneling across the metal/semiconductor junction. Spin injection experiments were conducted in a vertical LED device in Faraday geometry, where the degree of circular polarization of the emitted light is directly connected to the electron spin polarization in the active region. Interface mixing and spin polarization losses during the electrical transport in the GaN layer towards the quantum well detector are discussed in relation with the low value of the detected spin polarization.

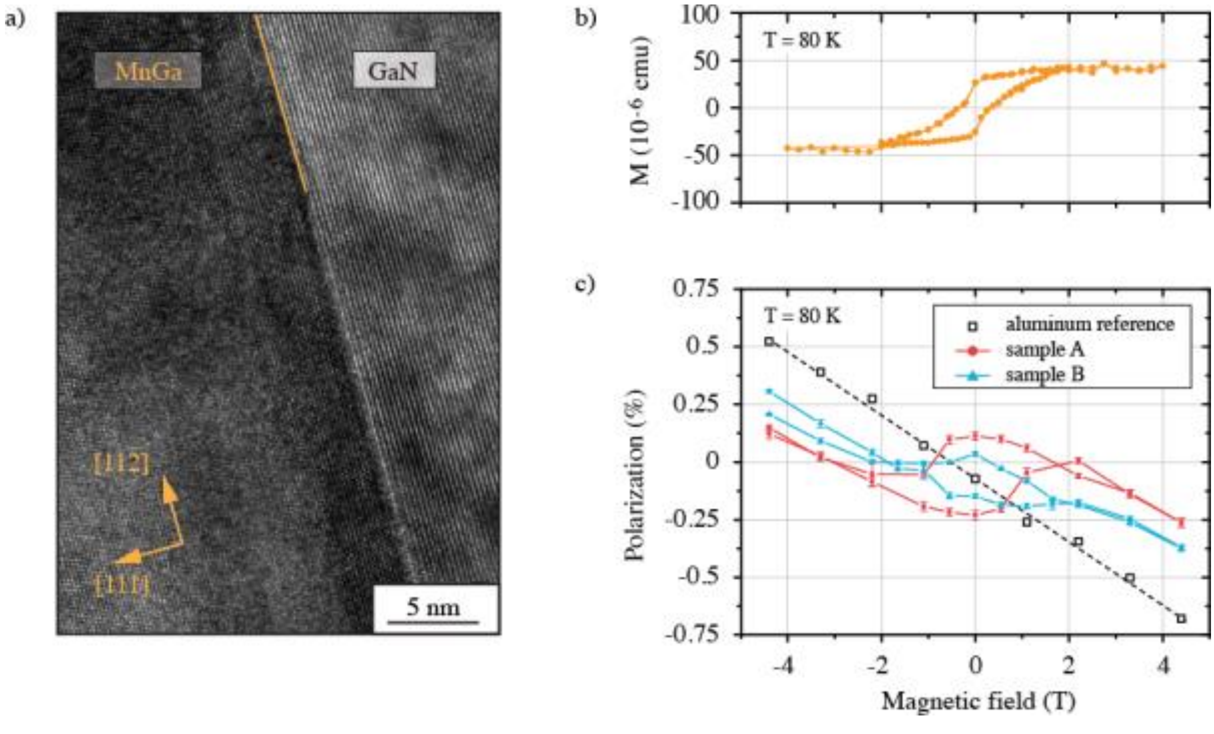

Figure 1: (a) A sharp MnGa/GaN interface is exhibited in the HR-TEM image, taken in the [-101] zone axis of MnGa. (b) VSM measurement of the magnetic moment of a 4x4 mm2 piece of LED sample B with the magnetic field applied out-of-plane. (c) Dependence of the optical polarization on the applied magnetic field, indicating a weak spin injection.

Ballistic Emission Electron Microscopy investigation of the spin filtering effect in epitaxial Fe/Au/Fe/GaAs(001) spin valve

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Ballistic Electron Magnetic Microscopy (BEMM) is a unique experimental tool allowing characterization of electronic properties of buried metal/semiconductor interfaces with nanometric lateral resolution [1]. In this communication, we will discuss experimental BEMM investigations on epitaxial Fe/Au/Fe/GaAs(001) spin-valves. In BEMM experiments, hot electrons are injected from an STM tip into the spin-valve/semiconductor heterostructure. The hot electron current is first modulated by the giant magnetoresistance effect in the spin-valve, and then energy and momentum-filtered at the epitaxial interface Schottky barrier [2].

The epitaxial Fe/Au/Fe/GaAs(001) structure presents a hot electron magnetoresistance (MR) as high as 500% at room temperature. This large MR amplitude is observed to be independent on the Fe layers thickness, and is thus dominated by interfacial effects. We demonstrate that these strong MR effects are related to a spin filtering effect at the gamma point, theoretically predicted by Autès et al [3]. Above the Schottky barrier height, hot-electrons are collected in the Γ valley of GaAs selecting thus only electrons with a close to zero transverse momentum. Among these $k_{\parallel} \approx 0$ states, conservation of the electron wave-function symmetry at the Fe/Au epitaxial interfaces additionally selects electrons with the Δ_1 symmetry. These Fe Δ_1 states are fully spin-polarized and are responsible for the observed high magnetocurrent in these heterostructures [4]. The magnetocurrent amplitude can be tuned by changing the effective mass of the Γ or X valley of the semiconductor substrate in $Al_xGa_{1-x}As$ alloys, i.e. by changing the aperture of the collimator in k-space, in good agreement with theoretical expectations. This study opens the way to achieve ultrahigh MR at room temperature by using k-space filtering in epitaxial spin-valves on semiconductors. The obtained large MR signal can further be used to perform sub-surface BEMM quantitative magnetic domain imaging with large contrast and nanometric lateral resolution [5].

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Topological phase, spin-orbit and exchange coupling induced in graphene under contact with heavy and magnetic metals

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Graphene is one of most perspective material in modern nanoelectronics due Dirac cone electronic structure at the K-point of the Brillouin zone. Recently a series of works appear in literature demonstrating enhanced induced spin-orbit (SO) coupling in graphene under contact with heavy metals. It allows to assume a practical realization of the topological phase formation predicted in graphene [1] with the energy gap at the Dirac point induced by SO coupling. It allows realization of the Quantum Spin and Anomalous Hall effects in graphene which are manifested in creation of the 1D-edge states in the open SO gap. In the present talk a possibility of an enhanced induced spin-orbit coupling in graphene and formation of corresponding topological phase in graphene under contact with heavy metals (Au, Ir, Pt, Pb) will be analyzed. In relation to it, the induced contributions of the intrinsic (internal) and extrinsic (Rashba-like) SO coupling realized in the studied systems and also the influence spin-dependent hybridization will be analyzed and estimated. The experimental investigation of spin and electronic structure was carried out by photoemission with angle and spin resolution, and crystalline structure of graphene synthesized on Pt(111), Ir(111) monocrystals and modified by intercalation of Pt, Au and Pb monolayers under the synthesized graphene was studied by STM and LEED. Comparison with theoretical calculations is carried out. As a result, we estimate a relation between the intrinsic and extrinsic contributions in the induced SO coupling in dependence on the mutual arrangement of graphene and metal atoms. It is shown that for graphene contacting with Au(111) and Ir(111) the Rashba-like contribution prevails in the induced SO coupling that is followed by the induced spin splitting up to 100-150 meV without the Dirac gap formation [2]. For graphene on Pt(111) [3] and for graphene on Ir(111) with intercalated Pt monolayer [4] a spin-dependent hybridization at the Fermi level plays significant role with comparable contributions of the intrinsic and extrinsic contributions, and for graphene on Pt(111) with intercalated Pb monolayer the SO gap at the Dirac point is observed [5] with the spin structure in the upper and lower Dirac cone predicted for topological phase. For comparison, the system with intercalated Cu monolayer where the gap at the Dirac point opens by the sublattice symmetry breaking is presented and analyzed. At the end a possibility of interplay between SO and exchange coupling and manipulation of the induced SO splitting in graphene by the induced magnetic moment is demonstrated in the system included both heavy (Au) and magnetic (Co) atoms.

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Band Alignments in Fe/Graphene/Si(001) Junctions Studied by X-ray Photoemission Spectroscopy

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The control of tunnel contact resistance is of primary importance for semiconductor-based spintronic devices [1]. This control is hardly achieved with conventional oxide-based tunnel barriers due to deposition-induced interface states. Manipulation of single 2D atomic crystals (such as graphene sheets) weakly interacting with their substrate might represent an alternative and efficient way to design new heterostructures for a variety of different purposes including spin injection into semiconductors [2].

We studied by x-ray photoemission spectroscopy the band alignments and interface chemistry of iron–graphene-hydrogenated passivated silicon (001) surfaces for a low and a high n-doping concentration. We found that the hydrogen passivation of the Si(001) surface remains efficient even with a graphene sheet on Si(001) surface. For both doping concentrations the semiconductor is close to flat-band conditions which indicates that the Fermi level is unpinned on the semiconductor side of the Graphene/Si(001):H interface [Fig. 3]. When iron is deposited on the graphene/Si(001):H structures the Schottky barrier height remains mainly unaffected by the metallic overlayer [3] with a very low barrier height for electrons, a sought-after property in semiconductor based spintronic devices.

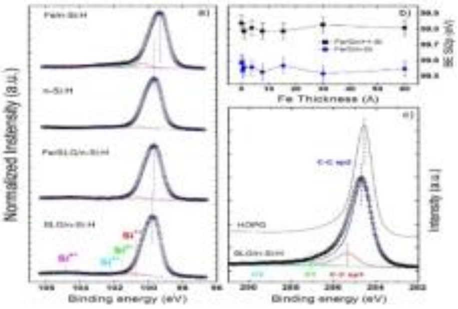

Fig. 4: (a) XPS spectra of Si2p core level for n-Si:H and SLG/n-Si:H before and after deposition of 15Å Fe. (b) Binding energy of the Si bulk component of the Si2p$_{3/2}$ core level for SLG/n-Si and n++-Si as a function of iron thickness. (c) XPS spectra of C1s core level of HOPG and SLG/n-Si:H.

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Temperature versus doping effects on low-energy plasmons in graphene

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Graphene which consists of a single layer of carbon atoms, is an ideal realization of a system in which electrons, confined in two dimensions, are quantum-mechanically enhanced. Moreover, recent advances in fabrication techniques for graphite structures now make it possible for such exotic two-dimensional (2D) electron systems to be probed experimentally. In graphene the collective quasiparticle phenomena giving rise to the plasmon excitation spectra may display interesting features [1,2] which are accessible experimentally [3-6]. Additionally, their behavior is expected to differ substantially from the well-understood plasmonic properties for quantum wells in conventional semiconductor heterostructures, including group-IV compounds, binary systems of group III-IV elements, metal chalcogenides, and complex oxides [7,8].

Here, we report on an *ab initio* theoretical investigation of the anisotropy of low-energy graphene plasmon excitations which may be induced by finite temperature in either the presence or absence of carrier doping. Adjusting the chemical potential with the use of an electric field effect, we observe how the 2D plasmon dispersion varies strongly with temperature and doping level. Also we predict existence at finite temperature of a second plasmon branch with acoustic anisotropic dispersion, like it was found for the finite doping [9]. We aim to compare what combination of temperature and doping corresponds suitably to doping only at T=0 K.

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Quantum Dots in Graphene Nanoribbons

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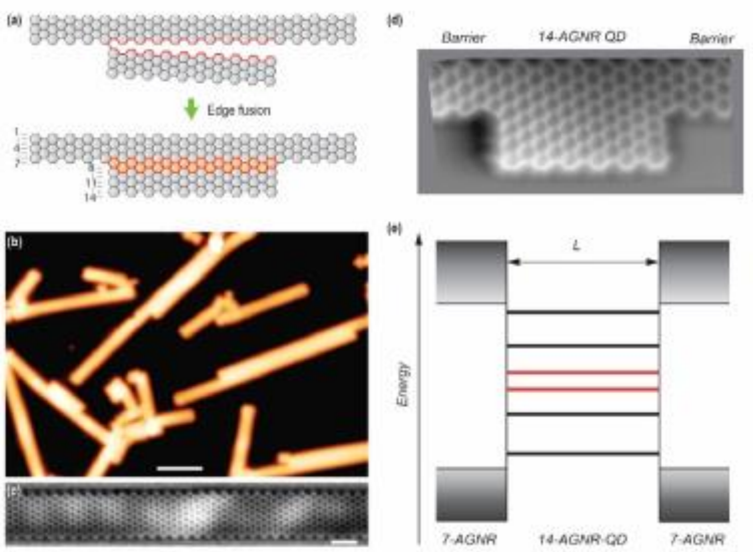
Recent advances in on-surface chemistry enable the fabrication of graphene nanoribbons (GNRs) with atomic precision, opening the door to tailoring their electronic properties to the needs of specific applications [1]. Here, we report the fabrication of widely tunable graphene quantum dots (GQDs) by creating GNR heterostructures that are achieved through edge fusion of armchair GNRs with a width of 7 C atom pairs (7-AGNRs) [2]. We show that the applied bottom-up fabrication approach yields atomic precision of the resulting 7-14-7 AGNR heterostructures not only in the width of the individual GNR segments but also at the interfaces separating them.

Based on scanning tunneling spectroscopy investigations, we have determined a sharp transition of the energy gap from 2.4 eV inside the 7-AGNR segments to 0.15 eV in the central 14-AGNR QD region. An in-depth understanding of electronic properties has been gained by comparison of differential conductance maps to combined density functional theory and tight binding calculations, which reveal the presence of a pair of low energy interface states at the atomically sharp 7-14 AGNR interfaces. The exponential dependence of the energy splitting of these interface states on the 14-AGNR QD length allows a wide tunability of the fundamental gap of the GQDs by one order of magnitude within few nanometers length range. In addition, non-contact atomic force microscopy images directly resolve the atomic structure of GQDs, giving unprecedented insight into the relation between atomic and electronic structure of the fabricated GQDs.



(a) Schematic illustration of the formation of a 14-AGNR quantum dot by edge fusion of two 7-AGNRs. **(b)** STM image showing several 7-14-7 heterostructures on Au(111). Scale bar: 5 nm. **(c)** nc-AFM frequency shift image of a long 14-AGNR segment. Scale bar: 2 nm. **(d)** nc-AFM image of a short 14-AGNR quantum dot. **(e)** Illustrated energy levels of the 14-AGNR quantum dot in (d). Two red lines indicate a pair of interface states, the black lines represent the levels arising from longitudinal quantum confinement of electrons in the 14-AGNR segment.

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Interplay of bond and site electron-phonon coupling in one dimension

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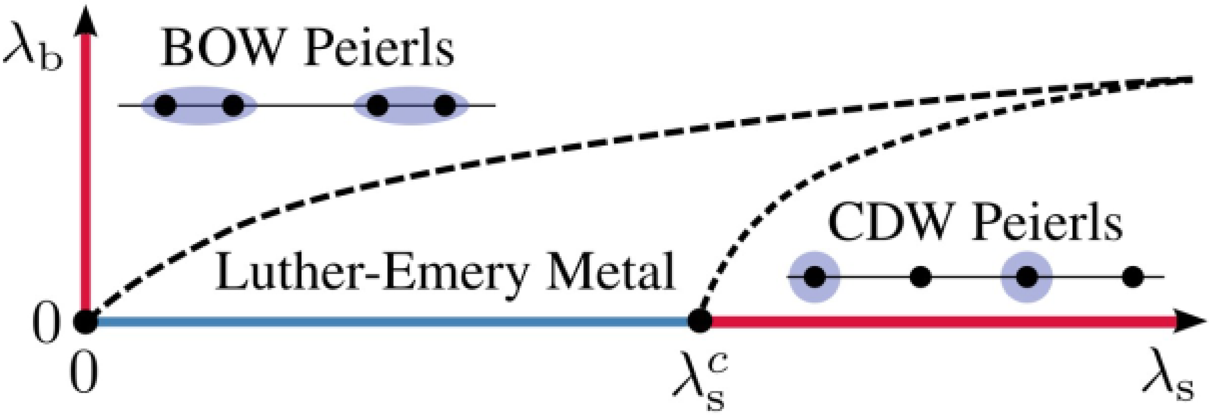
The interplay of bond and charge correlations is studied in a one-dimensional model with both Holstein and Su-Schrieffer-Heeger (SSH) couplings to quantum phonons. The problem is solved exactly by quantum Monte Carlo simulations. If one of the couplings dominates, the ground state is a Peierls insulator with long-range bond or charge order. At weak coupling, the results suggest a spin-gapped and repulsive metallic phase arising from the competing order parameters and lattice fluctuations. Such a phase is absent from the pure SSH model even for quantum phonons. At strong coupling, evidence for a continuous transition between the two Peierls states is presented.



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Pinning of topological solitons at extrinsic defects in a quasi-one-dimensional charge density wave

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Quasi one-dimensional (1D) electronic systems are known to exhibit exotic physical phenomena, such as, e.g., Jahn Teller distortions, charge density wave (CDW) formation and non-Fermi liquid behavior. Solitonic excitations of the charge density wave ordered ground state and associated topological edge states in atomic wires are presently the focus of increasing attention. We carried out a combined *ab initio* and scanning tunneling microscopy (STM) study of solitonic and non-solitonic phase defects in the In/Si(111) atomic wire array. While free solitons move too fast to be imaged directly in STM, they can become trapped at extrinsic defects within the wire. We discuss the detailed atomistic structure of the responsible extrinsic defects and trapped solitons. Our study highlights the key role of coupled theory-experimental investigations in order to understand also the elusive fast moving solitons. S. W. gratefully acknowledges financial support from the German Research Foundation (DFG), grant No. FOR1700.

One-dimensional metallic nanostructures on highly anisotropic silicon surfaces

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Physics of one dimensional objects attracts considerable attention because of its relative simplicity when considering theoretical description of various phenomena as compared to 2D and 3D systems. However, from the experimental point of view it is much more difficult to prepare one-dimensional structures of well-defined sizes than objects of higher dimensionality. In addition, it is usually required to get nanostructures which are well-isolated from a substrate on which they are formed. Such structures often have non-uniform width or, even if they have a form of perfect atomic chains, they are more or less strongly electronically coupled to a substrate.

Among a number of various methods, vicinal silicon substrates allow for self-organized growth and formation of (quasi) one-dimensional metallic structures. Such surfaces consists of atomically flat terraces separated from each other by steps. A terrace width, and therefore also a width of nanostructures and distance between them, can be easily tuned by an angle at which surface is cut with respect to a low Miller index plane. Regular distribution of steps over macroscopic size regions is usually obtained by deposition of submonolayer amount of gold which forms chains of atoms. There are many examples of such systems e.g. Si(557)-Au, Si(335)-Au or Si(553)-Au [1].

It has been demonstrated that regularly distributed one-dimensional structures on the vicinal Si substrates can also be obtained with Pb atoms [2, 3]. It appears that the Si(557)-Pb surface reveals Fermi nesting [4] or exotic spin-orbit density waves [5]. A very similar surface, Si(553)-Pb, reveals a pure one-dimensional character of Pb nanoribbons with electronic states which are very well decoupled from the Si substrate. In addition the Pb-induced surface states show a giant Rashba-type spin-splitting [6].

Motivated by their reach physics and a number of new phenomena observed in such systems we investigate different (quasi) one-dimensional metallic nanostructures prepared on highly anisotropic silicon surfaces: (553), (331) and (110). In this contribution we present and compare their basic crystallographic and electronic properties measured with reflection high energy electron diffraction, scanning tunneling microscopy and angle-resolved photoelectron spectroscopy techniques.

This work has been supported by the National Science Center under Grant No. 2013/11/B/ST3/04003

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Functionalization of Si(553)-Au surface with hydrogen and small organic molecules

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We propose to use atomic metallic chains deposited on vicinal Si substrates as templates for the growth of hybrid molecule-solid nanostructures. The advantage of these substrates is the possibility to vary the substrate geometry and the metallic element, leading to a family of surfaces with a broad spectrum of potential applications in organic electronics and bio-sensing. We investigate the adsorption of toluene-3,4-dithiol molecules on hydrogen-passivated Si(553)-Au surfaces as model system/process. Additionally, hydrogen is able to drive a reversible metal-insulator transition on the Si(553)-Au surface and is also changing the adsorption geometry of organic molecules[1], extending the functionalization possibilities of the surface.

Our approach for investigating molecule adsorbtion consists in establishing a direct connection between optical spectra and surface structure via ab-initio calculations[2]. Optical spectra and their theoretical interpretation allow us to gain information on structural and electronic properties of the system. We use a set of surface-sensitive and polarization-sensitive optical techniques, such as Raman Spectroscopy (RS), Reflection Anisotropy Spectroscopy (RAS) and Infrared Spectroscopic Ellipsometry (IRSE).

The understanding of charge transfer between molecules and atomic wires in highly ordered molecular arrays is crucial for the realization of further functionalization through modification of terminal groups of molecules.

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What we can learn from plasmons in gold induced wires on Si(hhk)

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For future plasmonic devices, the understanding of low-dimensional collective excitations is indispensable. Nevertheless, although fundamental theories of the properties of low-dimensional plasmons exist for many years, their predictions of the behavior are still rather unsatisfactory. Several key aspects of the influences in real world systems such as, e.g., many-body effects, Coulomb screening, as well as the general impact of the surrounding structural elements are still rather unexplored. Furthermore, quasi-one-dimensional electronic systems show exceptional transport properties such as Peierls transition or Tomonaga-Luttinger liquid (TLL) behavior that may have a strong influence on the plasmonic properties.

For the investigations, the wire quality was checked with spot profile analysis in low energy electron diffraction (SPA-LEED). A combination of an electron energy loss spectrometer (EELS) and SPA-LEED providing both high energy and momentum resolution gave access to the plasmon dispersion.

As quasi-one-dimensional structures, Au-induced wires on regularly stepped Si(hhk) offer the perfect playground for systematic investigations with their varying terrace widths. Therefore, in the first part of this work, the systems were prepared to a state, where each of these terraces hosts a gold chain of either single or double atomic width. Although 1D metallicity is observed, the plasmon dispersion strongly depends on two-dimensional crossover. On the one hand, this crossover is caused by the feedback of the spacing of the wires, a so-called interwire correlation. On the other hand, the distribution of the 1D electronic band structure is both affected by the terrace width as well as by the additional structural elements. Modifications of a quasi-free electron gas plasmon model including calculated electronic band structures were able to describe the observed plasmon dispersions qualitatively. Widths of the plasmon loss peaks revealed broadening beyond merely an effect of the lifetime. Adsorption measurements with molecular oxygen and atomic hydrogen showed the possibility to change the energy of the plasmons. Though their changes were counterintuitive with an increase of the energy upon oxygen adsorption and a decrease by hydrogen, the introduced modified model can explain this behavior by changes in their band structures.

Probing non-equilibrated Dirac fermions on surface 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. Here, the surface Dirac fermion dynamics in the "carrier tuned" topological insulator $(Sb_{1-x}Bi_x)_2Te_3$ have been explored by time- and angle-resolved photoelectron spectroscopy implementing pump-probe method that enables us to observe not only occupied/unoccupied electronic states but also carrier dynamics. The experiment was carried out with linearly polarized pump ($h\nu$=1.48 eV) and probe (5.92 eV) pulses generated by Ti:sapphire laser system operating at a repetition rate of 250 kHz [1]. Sb_2Te_3 (x=0) has a Dirac node completely located above the Fermi energy [Fig.1(a)]. 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 gap by an appropriate Bi doping (x=0.43) as shown in Fig.1(a), 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 [Fig.1(b)] [3]. We have also observed a downward (an upward) surface photovoltage shifts in n-type (p-type) sample of Bi_2Te_3 [4]. These findings expand the pathways to high-mobility opto-spintronic applications.

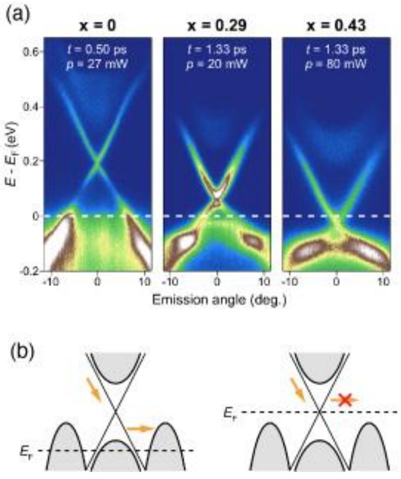

Figure 1: (a) Band dispersions acquired at certain pump-and-probe delay times. (b) Schematics of the relaxation processes in bulk metallic and bulk insulating TIs.

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Edge states at topological crystalline insulator surfaces: a new approach towards robust 1D modes

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Topological crystalline insulators (TCIs) are topological materials where the existence of surface Dirac states is guaranteed by crystal symmetries. This protection mechanism promises a rich phenomenology in response to crystal perturbations. In my presentation, I will report on the discovery of robust 1D spin-polarized channels naturally emerging at TCI surfaces once translational invariance is broken [1]. I will illustrate how 1D channels can be easily obtained in the prototypical TCI Pb1−*x*Sn*x*Se without the need of any sophisticated preparation technique. In particular, by correlating topographic and electronic structure information, I will show that 1D states naturally emerge at step edges consisting of an odd number of atomic layers, where translational invariance is broken, while even step edges maintain translational symmetry and are featureless. By systematically acting on the crystals stoichiometry, I will demonstrate how these 1D states are directly linked to the existence of a topologically non-trivial bulk band structure. A minimal toy model and realistic tight-binding calculations allow to identify them as spin-polarized at bands connecting two Dirac points. Finally, I will show how, contrary to 1D topological states known so far, their protection mechanisms result in a striking robustness to defects, strong magnetic fields, and elevated temperature.

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Scrutinizing the III-V-on-Si interface formation on the atomic scale *in situ* and by DFT

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III/V-on-Si integration is highly relevant for for microelectronics, photovoltaics, and water-splitting. A pseudomorphic virtual GaP/Si heterointerface is of particular interest since its atomic and electronic structure impacts crystal quality directly. Well-ordered interfaces are desirable but the formation of polar-on-nonpolar heterointerfaces is not yet fully understood. It is instructive to control each of the three steps (i) Si surface formation, (ii) III/V nucleation, and (iii) III/V layer growth individually *in situ*, which largely benefits from complementary surface science techniques as well as density functional theory (DFT). Here, we will highlight how such a combination enables specific metalorganic vapor phase (MOVPE) preparation of virtual substrates for both (100) and (111) orientation. Kinetics and energetics, which govern Si surface processes, highly depend on the misorientation of the substrate: Large Si(100) terraces may be object to Si layer-by-layer removal upon annealing in H2 ambient, while the same kinetics can be utilized for the preparation of energetically unfavorable A-type terraces. Formation of the heterointerface at elevated temperature depends on numerous aspects, such as preferred binding sites, atom mobility, step height, and density, as well as process routes. Quantitative XPS revealed about one ML of Si—P bonds at the interface, which implies a kinetically limited interface structure that is “frozen” during further processing [2]. For nucleation in more Ga-rich ambient, the prevailing GaP sublattice grows inverted, which is in line with DFT predicting that Si—Ga bonds become more favorable with increasing Ga chemical potential for abrupt interfaces [1]. We also find interface states in the common band gap above the VBM [3]. Their predicted dispersion is anisotropic and provides distinct features for further experimental investigation. Controlled modification of the Si surface with As prior GaP growth enables inversion of the GaP sublattice orientation both on Si(111) [4] and Si(100) [5]. XPS indicates that the heterointerface is less abrupt than in the As-free case. The sublattice inversion is particularly useful for GaP/Si(111), where P-polarity is essential for subsequent nanowire growth [5], and a dedicated GaP nucleation process allows for efficient suppression of rotational twins [6].

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Determination of electronic and atomic properties of surface, bulk and buried interfaces: Simultaneous combination of hard X-ray photoelectron spectroscopy and X-ray diffraction

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Hard X-ray photoelectron spectroscopy (HAXPES) is a powerful novel emerging technique for bulk compositional, chemical and electronic properties determination in a non-destructive way. It benefits from the exceptionally large escape depth of high kinetic energy photoelectrons enabling the study of bulk and buried interfaces up to several tens of nanometres depth. Its advantage over conventional XPS is based on the long mean free path of high kinetic energetic photoelectrons. Using the advantage of tuneable X-ray radiation provided by synchrotron sources the photoelectron kinetic energy, i.e. the information depth can be changed and consequently electronic and compositional depth profiles can be obtained. The combination of HAXPES with an atomic structure sensitive technique, as X-ray diffraction, opens a new research field with great potential for many systems in which their electronic properties are intimately linked to their crystallographic structure. At SpLine, the Spanish CRG Beamline at the European Synchrotron Radiation Facility (ESRF) we have developed a novel and exceptional set-up that combine grazing incidence X-ray diffraction (GIXRD) and HAXPES. Both techniques can be operated simultaneously on the same sample and using the same excitation source. The set-up includes a heavy 2S+3D diffractometer and UHV chamber equipped with an electrostatic analyzer. The UHV chamber has also MBE evaporation sources, an ion gun, a LEED optic, a sample heating and cooling device, an electron gun, a UV discharge lamp, a low and medium energy X-ray tube, leak valves and a load-lock port. The photon energy ranges between 7 and 45 keV. The HAXPES analyzer is an electrostatic cylinder-sector (FOCUS HV CSA), with a compact geometry and high transmission due to second order focusing. The analyzer is capable to handle kinetic energies both up to 15 keV and down to a few eV with the same analyzer setup and power supply. In this contribution we will describe the experimental set-up together with an overview of the excellent capabilities of the proposed experimental techniques for the detailed characterization of surfaces and buried interfaces. Selected examples will be presented.

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Work function measurements of bilinear self-assembled monolayer arrays: The role of electrostatic potentials for Ultraviolet Photoelectron Spectroscopy

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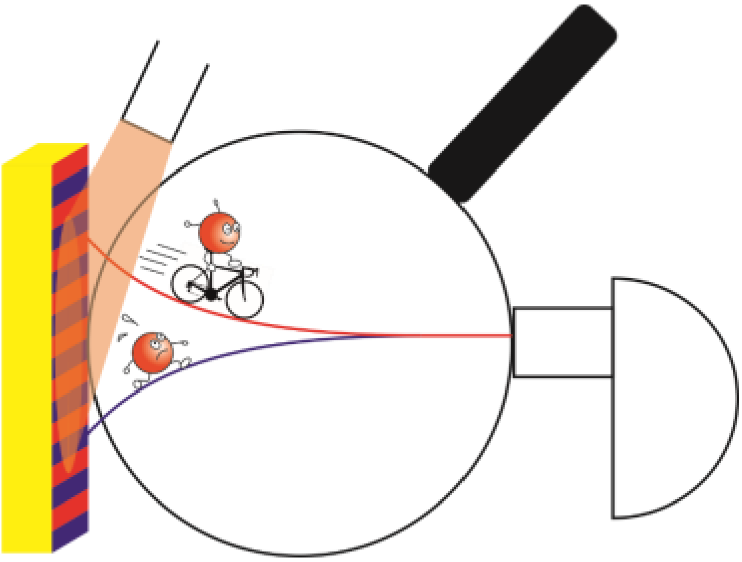
Ultraviolet photoelectron spectroscopy (UPS) is one of the primary techniques to determine the work function of surfaces. Heterogeneous surfaces are expected to exhibit one secondary electron cut-off (SECO) representing an averaged sample work function. However, a vast number of reports has shown that more than one cut-off can be observed for heterogeneous surfaces. To clarify this discrepancy, a heterogeneous model system consisting of bilinear arrays of two self-assembled monolayers (SAMs), providing a periodic work function pattern with a difference of more than 1 eV, is investigated. With UPS two SECOs are measured, one reflecting the high work function SAM and the other an averaged work function. To explain these observations, the electrostatic potential above the surface is investigated by Kelvin-Probe Force Microscopy (KPFM) and compared to electrostatic modeling. We unravel quantitatively that the electrostatic potential from the high work function areas leads to an additional energy barrier for the electrons emitted from the low work function areas and show further the influence of measurement parameters. The reported findings are important for accurate interpretation of work function measurements by UPS.



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Resonant Raman scattering at surface vibrational modes of clean and O-terminated Cu(110)

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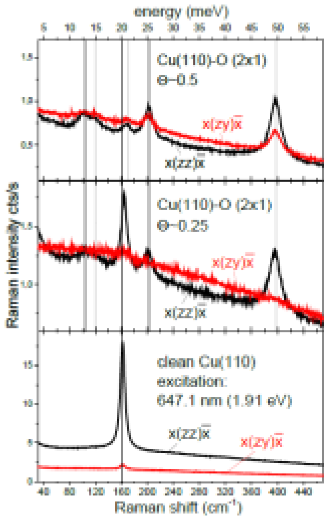
In recent years Raman spectroscopy has been successfully employed to study surface vibrational modes of semiconductors via surface resonant Raman scattering. Metals like Cu, Ag, Au, on the other hand, which are important substrates for Surface Enhanced Raman scattering from rough surfaces, are not expected to show Raman signals from first order scattering at phonons, due to their crystal structure. Therefore, it is of particular interest that our surface Raman experiments show for the first time that the symmetry breaking on the metal surface enables inelastic light scattering from surface phonon modes. As it is known from inelastic electron and He atom scattering the clean Cu(110) as well as the O-terminated (2x1) Cu(110) surfaces exhibit characteristic sets of surface vibrational modes. Surface Raman spectroscopy enables now high spectral resolution measurements of this set of surface vibrational modes and a determination of their intrinsic lifetimes.

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. 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. We demonstrate that surface electronic states play a crucial role in the Raman scattering mechanism: Surface vibrational modes are observed under resonant scattering conditions to surface electronic transitions. By lattice vibrational calculations we are able to identify surface phonons and surface resonances of the clean and O-terminated surface which show up as strong peaks in the respective Raman spectra.



Raman spectra of clean and O-covered Cu(110) for different light polarization

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Multi-layered waveguide silicon structure for solar cells models

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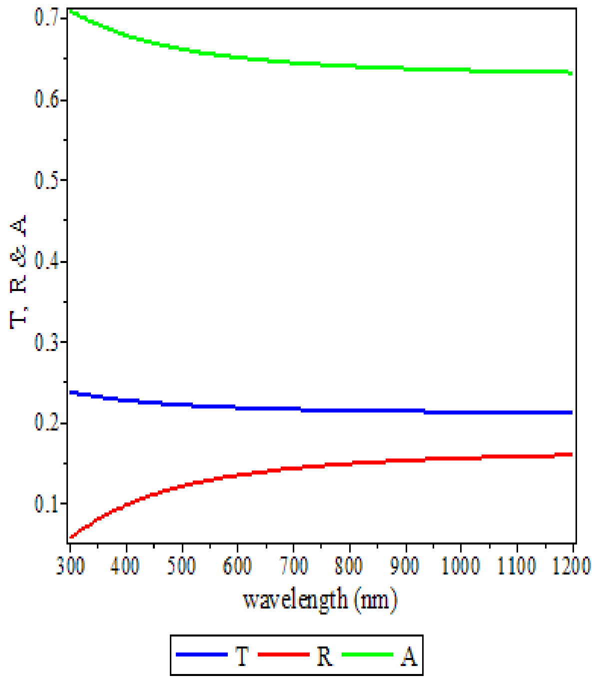
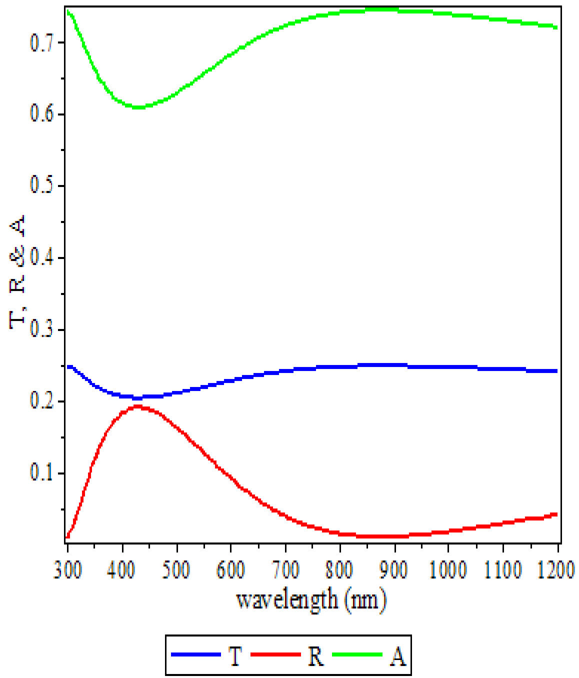
Abstract

In this paper, the optical proprieties of multilayer photonic structures with several semiconductors for silicon solar cell are studied. Despite its favorable electronic, physical, and chemical properties, silicon remains a poor absorber. The losses due to the reflection at the air/glass interface is another disadvantage, which limit the efficiency of the solar cell. To ameliorate the optical absorption of the previous conventional antireflective structures, we propose photonic structures formed by semiconductors double layers such as SiO_2/TiO_2. The transfer matrix method is used to derive the transmission and reflection coefficients. The application of the law of conservation of energy allowed the determination of the absorption coefficient. From a comparison between the optical parameters of these structures and the conventional antireflective structures at normal incidence, an improvement of the absorption is observed for appropriate thicknesses. The effect of the incidence angles is also discussed.



Transmission, Reflection and Absorption coefficients at normal incidence versus the wavelength (conventional antireflective structure SiO_2/TiO_2)



Transmission, Reflection and Absorption coefficients at normal incidence versus the wavelength (photonic structure with three pairs SiO_2/TiO_2)

Low temperature plasma epitaxy of Silicon on III-V for tandem solar cells

G. Hamon[1,2] , N. Vaissiere[1], R. Cariou[1,3], W. Chen[1], M. Foldyna[1], R. Lachaume[4], J. Alvarez[4], J. L Maurice[1], J. Decobert[3], J.P. Kleider[4] and Pere Roca i Cabarrocas[1]

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Integration of III-V materials on silicon has been and still is a challenging subject due to lattice and thermal mismatch effects, as well as to the polarity issues at the interface which result in a high density of defects. To overcome these difficulties, we present here an original approach called inverted metamorphic growth where silicon is epitaxially grown on GaAs by low temperature plasma-enhanced CVD (PECVD). Without the need for ultra-high vacuum and keeping the substrate temperature around 200°C, both a GaAs surface cleaning and a subsequent heteroepitaxial growth were achieved and monitored by in-situ spectroscopic ellipsometry. The good electronic quality of the low temperature epi-Si and epi-SiGe layers has been demonstrated by making heterojunction solar cells on highly doped c-Si substrates [1]. This approach has been applied to the epitaxial growth of silicon on GaAs [2]. Aiming at tandem devices, we have also fabricated hybrid tunnel junctions where we combine low temperature RF-PECVD for Si and metalorganic vapour phase epitaxy (MOVPE) for GaAs. The electrical properties of these heterojunctions are measured and compared to that of a reference III-V tunnel junction. The presence of atomic hydrogen during the epi-PECVD of silicon on GaAs strongly reduces the doping level at the surface of GaAs. Indeed, 30 seconds of H_2 plasma exposition at 175 °C are sufficient to reduce the GaAs film doping level from 1.10^{20} cm^{-3} to less than 2.10^{19} cm^{-3} at the surface and over a depth of about 20 nm. However, the doping level can be fully recovered after annealing at 350 °C. Finally, optical and electrical modelling was used to optimize tandem GaAs/epi c-Si tandem solar cells [3].

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3. R. Lachaume, R. Cariou, J. Decobert, M. Foldyna, G. Hamon, P. Roca i Cabarrocas, J. Alvarez, and J.-P. Kleider : "Performance analysis of AlGaAs/epi-Si(Ge) tandem solar cells: a simulation study". Energy Procedia **84** (2015) pp. 41-46.

Radio-frequency scanning tunneling microscopy on molecular and atomic resonators

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To benefit from, both, the high spatial resolution (~Angstrom) of scanning tunneling microscopy (STM) and the exceptional energy resolution (< μeV) of magnetic resonance techniques, we have developed a spectroscopic radio frequency (rf) STM system with a bandwidth of presently about 4 GHz. Our method enables the detection and excitation of mechanical [1,2] as well as spin [3,4] degrees of freedom in single (individual) functional molecules adsorbed on solid surfaces at cryogenic temperatures, maintaining sub-nanometer real-space resolution. My contribution surveys recent showcases of rf-STM by my group. I'll report on concerted mechanical oscillations of weakly coupled pi-radical molecules in the 100 MHz regime at 30 K as well as the resonant excitation of single nuclear (I) and electronic (J) spins up to 4 GHz in individual molecular quantum dots at 5 K [3,4]. The latter are formed by individual molecules of the single-molecule magnet bis-phthalocyanato-terbium(III). The observed single-spin excitations involve I=3/2 and J=6, respectively, and occur unbound from electromagnetic dipole selection rules, i.e. exhibiting $\Delta I_z = \pm 3$ and $\Delta J_z = \pm 12$, which can be explained by a spin-phonon-like excitation mechanism [5]. I'll end my presentation with a preliminary outlook on the role of rf-induced plasmonic surface excitations, which becomes observable by our method with the help of physisorbed noble gas atomic clusters.

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Molecular Orbital Rule for Quantum Interference in Weakly Coupled Dimers: Low-Energy Giant Conductivity Switching Induced by Orbital Level Crossing

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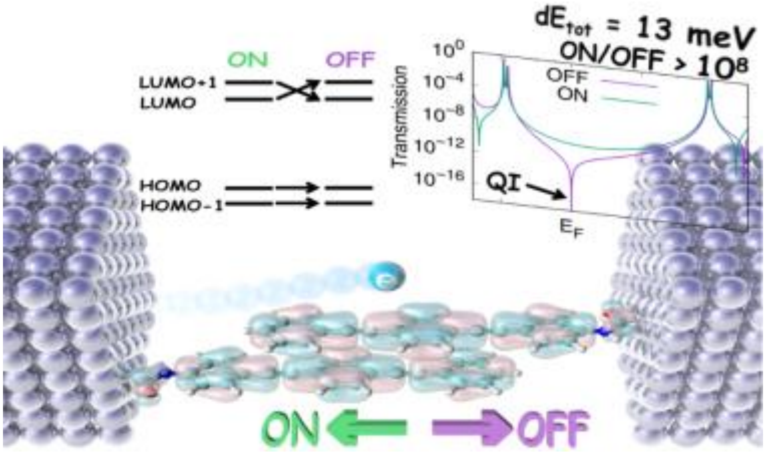
Destructive quantum interference (QI) in molecular junctions has attracted much attention in recent years. It can tune the conductance of molecular devices dramatically, which implies numerous potential applications in thermoelectric and switching applications [1]. There are several schemes that address and rationalize QI in single molecular devices. Dimers play a particular role in this respect because the QI signal may disappear, depending on the dislocation of monomers [2,3]. We derive a simple rule that governs the occurrence of QI in weakly coupled dimer stacks of both alternant and nonalternant polyaromatic hydrocarbons (PAHs) and extends the Tada-Yoshizawa scheme [4,5]. Starting from the Green's function formalism combined with the molecular orbital expansion approach, it is shown that QI-induced antiresonances and their energies can be predicted from the amplitudes of the respective monomer terminal molecular orbitals [6]. The condition is illustrated for a toy model consisting of two hydrogen molecules and applied within density functional calculations to alternant dimers of oligo(phenylene-ethynylene) and nonalternant PAHs. Minimal dimer structure modifications that require only a few millielectronvolts and lead to an energy crossing of the essentially preserved monomer orbitals are shown to result in giant conductance switching ratios.



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Resonance phenomena in ferrocene-based single-molecule junctions

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Ferrocene dithiol (FDT) molecules as molecular junctions and switches are particularly attractive because of their high conductance and their rotational flexibility. In our study of electrical transport through single FDT molecules between Au contacts via the break junction technique it turns out that the conductance depends strongly on the chemical end groups. This dependence allows tuning of the energy level alignment of HOMO and LUMO relative to the Fermi energy of the electrodes, as demonstrated by the comparison between ferrocene-1,1 ′-diamine (FDA) and FDT, making FDT a much better conductor than FDA. Comparison of the experimental results with DFT calculations based on the single level model suggest changes of binding geometries of the molecule at the electrodes as a function of electrode separation for both molecules. Particularly interesting are resonances in the IV-curves of FDT at fixed contact distances in the conductance range (at zero bias) between 0.09 G_0 to 0.5 G_0, which are symmetric with respect to the applied bias voltage. This structure is absent for zero bias conductances above as well as below these limits and shifts systematically with decreasing zero bias conductance from 25 to 30 mV at the highest conductances to 120 mV at 0.09 G_0. While vibrationally assisted inelastic transport processes can be excluded to describe this phenomenon, it is more compatible with the Fano resonance model, as verified for selected molecular binding geometries in DFT simulations, which, however yields a too high temperature dependence.

A microscopic view of atomic and molecular contacts

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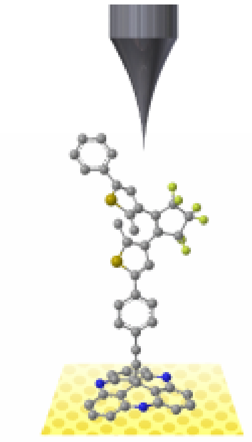
The electron transport through single atoms and molecules is investigated with low-temperature scanning probe microscopy. In the experiments, which aim at maximizing the control over the junction properties, the conductance and the acting force are probed. The talk will address the magnetoresistance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

Support via SFB 668 and 677 is acknowledged.



Emergence of topologically non-trivial phases in systems consisting of the structure elements of layered giant-Rashba band insulators

S.V. Eremeev,[1,2,3,4,*] I.A. Nechaev,[2,3,5] E. E. Krasovskii,[4,5,6] P. M. Echenique,[4,5] and E.V. Chulkov[2,3,4,5]

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The BiTeX (X = I,Br,Cl) semiconductors have attracted considerable interest because of giant Rashba-type spin-orbit splitting in their bulk and surface electronic states [1–6] arising from a strong spin-orbit interaction and the material polarity. In addition to giant bulk and surface Rashba splitting a single BiTeX trilayer (TL) holds the Rashba-split state itself [7]. Among BiTeX, the BiTeI compound has the biggest Rashba interaction strength. The strong atomic spin-orbit coupling and a negative crystal-field splitting of the bands [7] have also been predicted to promote a topological insulator (TI) phase in BiTeI under external pressure [8]. Besides, the BiTeX semiconductors and their thinnest films, TLs, are promising to construct heterostructures containing topological insulators and BiTeX layers [7, 9]. In these heterostructures the interplay of topology and Rashba spin-orbit interaction may give rise to new electronic states and spin-dependent excitation phenomena. Recently we demonstrated that 2D TI phase can be realized in ultra-thin films built out of two inversely stacked noncentrosymmetric BiTeI trilayers, forming a centrosymmetric sextuple layer. This nontrivial sextuple layer turns out to be the structure element of an artificially designed strong 3D topological insulator $Bi_2Te_2I_2$ [10]. Next we have expanded our study to other BiTeX compounds, X = Br, Cl, constructing respective sextuple layers and bulk phases $Bi_2Te_2Br_2$ and $Bi_2Te_2Cl_2$. We have shown that $Bi_2Te_2Br_2$ bulk is 3D topological insulator while its thin films are trivial insulators. At the same time $Bi_2Te_2Cl_2$ is trivial band insulator in both 2D and bulk phases.

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Quantum spin Hall conductivity in 2D crystals

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The quantum spin Hall (QSH) phase is a quantum state of matter, proposed to exist in two-dimensional (2D) semiconductors with inverted band structure and, hence, a character of a topological insulator (TI). Such a quantum phase should exhibit a quantized spin Hall conductance but a vanishing charge Hall conductance. Since no external magnetic field is present, it can be only realized in materials with strong spin-orbit interaction (SOI). Indeed, indirect indications of the QSH phase have been observed for HgTe layers above a critical thickness.

We investigate as central quantity the (frequency-dependent) spin Hall conductivity $\sigma_{xy}^{sH}(\omega)$ by means of *ab initio* calculations using the relativistic electronic structures [1] of infinite 2D sheet crystals. As model systems we study slightly buckled, graphene-like atomic layers made by group-IV elements, silicene, germanene (Ge), and stanene, and their chemically functionalized, e.g. hydrogenated (GeH) or iodinized (GeI), counterparts. The sheet crystals are characterized by the Z_2 topological invariant. Numerical results are given for atomically thin Ge-based systems [2]. The influences of chemical modification, resulting topology, additional quantization, and topological edge states are discussed.

The inverted band structure of germanene with a fundamental gap due to SOI is strongly modified by its functionalization with I or H. As a consequence, we observe drastic changes in the frequency dependence of $\sigma_{xy}^{sH}(\omega)$. For germanene and GeI the static spin Hall conductivity exhibits quantization with e^2/h, the reciprocal von Klitzing constant, while its value is zero for GeH as shown in Fig. 1 [1,2]. These values are hardly influenced by temperature and Fermi level shift. The quantization is directly correlated with Z_2=1 or 0. For iodinized germanene nanoribbons we demonstrate that surprisingly the edge states slightly destroy the quantization.

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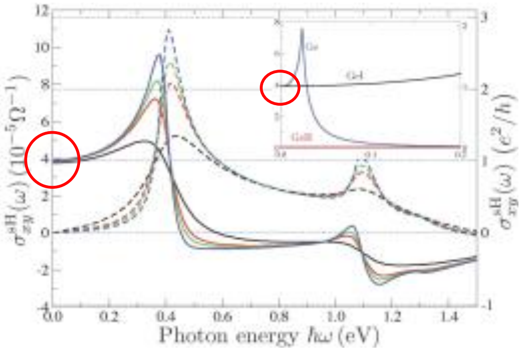

Figure 1: Real (solid line) and imaginary (dashed line) part of the spin Hall conductivity of GeI for different broadenings. The inset compares the results for GeI with those of Ge and GeH.

Spin-resolved and angular-resolved photo-emission spectroscopy experiments on in-situ transferred epitaxial Bi2Se3 thin films

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Topological insulators Bi2Se3 thin films with (0001)-orientation have been grown by Pulsed Laser Deposition on (111)-SrTiO3 and (0001)-Al2O3 substrates. The effects of the substrate temperature (ranging from 270°C up to 400°C) and the background pressure (ranging from 10-5 mbar to 10-1 mbar) on the structural properties of the Bi2Se3 films have been investigated. X-ray diffraction investigation demonstrates that epitaxial Bi2Se3 with single (0001)-orientation can be obtained on both substrates in a narrow (i.e. 20°C) range of deposition temperatures at 10-1 mbar of background pressure. In order to perform Spin and Angle-Resolved Photo-Emission Spectroscopy (SARPES) experiments, the sample surface quality has been checked by mean of in-situ Low-Energy Electron Diffraction (LEED), which showed that only films grown on (001)-Al2O3 substrates show an almost-unique in-plane orientation.

Spin-resolved and conventional ARPES experiments on the topological surface state of Bi2Se3 thin films, in-situ transferred directly from the PLD growth chamber, were performed by using synchrotron radiation. ARPES band dispersion of the Bi2Se3 thin films show a single Dirac cone, fingerprint of the topological surface states, centered at the Γ point. The spin-resolved spectra with the respective polarization are ascribed to the corresponding points of the k-space. Opposite spin polarization for opposite momenta have been found, confirming the fingerprint of the topological surface states, whose spin helical texture is strictly linked to the crystal momentum in the topological surface state.

Electrical resistance of individual defects at a topological insulator surface

Felix Lüpke, Markus Eschbach, Tristan Heider, Martin Lanius, Peter Schüffelgen, Daniel Rosenbach, Nils von den Driesch, Vasily Cherepanov, Gregor Mussler, Lukasz Plucinski, Detlev Grützmacher, Claus M. Schneider, and Bert Voigtländer

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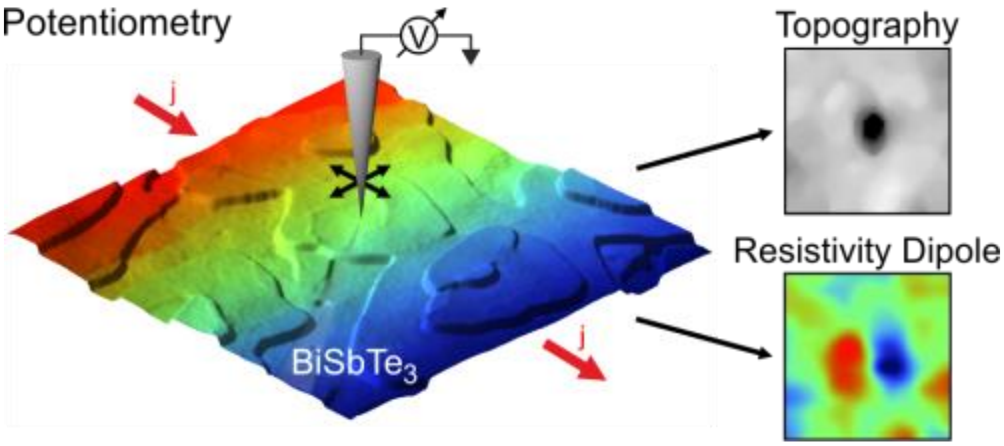
We determine the resistance of different kinds of defects at the surface of a $(Bi_{0.53}Sb_{0.47})_2Te_3$ topological insulator thin film by scanning tunneling potentiometry. The largest localized voltage drop we find to be located at domain boundaries in the topological insulator film, with a resistivity about four times higher than that of a step edge. Furthermore, we resolve resistivity dipoles located around voids in the sample surface. The influence of such defects with a typical diameter of 5 nm on the resistance of the topological insulator is analyzed by means of a resistor network model. Here, we show that local changes in the conductivity, e.g. due to the voids in the surface, give rise to a persistent voltage drop across the sample far away from the actual position of the defect. Due to the small size and the low density we find the resistance associated with the voids is miniscule compared to the resistance of the other surface defects.



Scanning tunnelling potentiometry at a topological insulator surface. Local voltage drops at step edges and domain boundaries and resistivity dipoles at void defects are observed.

Disentangling *in* situ top and bottom conductance of a topological insulator thin film

Felix Lüpke, Sven Just, Markus Eschbach, Tristan Heider, Martin Lanius, Peter Schüffelgen, Daniel Rosenbach, Nils von den Driesch, Vasily Cherepanov, Gregor Mussler, Lukasz Plucinski, Detlev Grützmacher, Claus M. Schneider, and Bert Voigtländer

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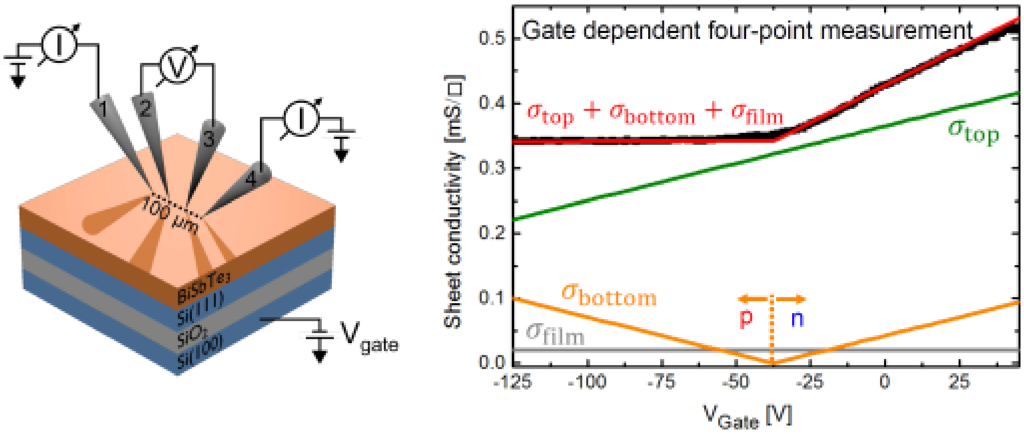
Charge transport in thin films of 3D topological insulator materials can be through the top and the bottom topological surface state as well as through the interior of the film. The latter undesirable conductivity can be minimized by the use of thin films (10 nm) and the use of MBE grown ternary material systems with reduced bulk conductivity. However, it is still difficult to separate the contributions of the three channels to the conduction. Using a multi-tip STM we performed *in situ* gate-dependent four-probe conductivity measurements of $(Bi_{0.53}Sb_{0.47})_2Te_3$ thin films. Combining the information from these measurements with the band structure obtained from subsequent ARPES measurements, we determine the carrier densities as well as the mobilities in the top and bottom topological surface state channels.



In situ gate-dependent four-probe conductivity measurements of $(Bi_{0.53}Sb_{0.47})_2Te_3$ thin films performed with a multi-tip STM.

Realization of Bismuthene – A Novel Two-Dimensional Material as High-Temperature Quantum Spin Hall Candidate

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Quantum spin Hall materials promise revolutionary devices based on dissipationless spin currents in conducting edge channels. However, for current systems such as HgTe the decisive bottleneck, preventing applications, is the small bulk energy gap of less than 30 meV, requiring cryogenic operation temperatures. To address this challenge, we have embarked in the epitaxy of ultrathin monoelemental topological insulators. A milestone has been the successful synthesis of the topological insulator □-Sn in our laboratory [1].

In specifically addressing the 2D regime, we have introduced SiC(0001) substrates as a growth template. This allows to realize lattice parameters for the overlayer which can be expected to host graphene-like hexagonal layers of Sn ("stanene") and Bi ("bismuthene"). As a prerequisite, we have shown the technological possibility to perform epitaxy on hydrogen-etched SiC of superior quality [2], and subsequent controlled atomic-scale growth [3].

In our current study we report the first successful epitaxy of a monolayer of bismuthene on SiC(0001). By combining experiment and theory we demonstrate that this material combination represents a new quantum spin Hall paradigm. In contrast to the previous mechanisms at work in both low-temperature quantum spin Hall materials graphene and HgTe, respectively, our approach specifically exploits the on-site atomic spin-orbit coupling as a third avenue. Consistent with theory, we detect a huge bulk gap of ~0.8 eV and conductive edge states [4]. Our results demonstrate a concept for a quantum spin Hall wide-gap scenario, where the chemical potential resides in the global system gap (including the insulating substrate). By virtue of the large bulk energy gap, this ensures robust conductance exclusively through the edge channels, and renders bismuthene suitable for the room-temperature regime.

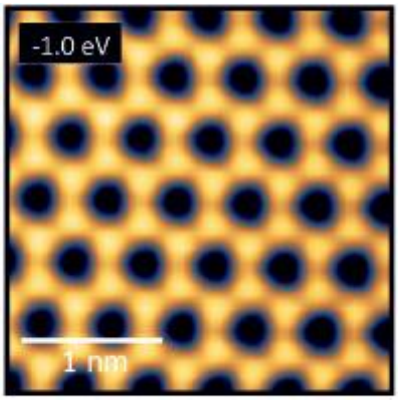

Fig. 1. Hexagonal lattice of bismuthene on SiC(001) as seen by scanning tunneling microscopy.

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Posters

Towards a Renewable Modified Surface for Rapid Sensing and Chelation of Heavy Metal ion Pollutants

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Heavy metal ion (HMI) pollutants are a threat to fresh water supplies and marine ecosystems [1]. Copper (Cu) can be highly toxic especially to aquatic ecosystems [2]. Silicon (Si) is an abundant material on the earth's crust and coupled with its semiconducting properties, it can also permit development of sensors that exploit ligand-analyte interactions. Electrochemical grafting of aryl diazonium derivatives have successfully been used to introduce various organic functional groups onto metallic or semiconducting surfaces [3]. The scope of this study was to introduce carboxymethylthio ligand groups via direct electrografting of 4-[(carboxymethyl)thio] benzenediazonium salt onto Si surfaces for chelation of Cu as initial steps towards creating a model renewable surface for sensing and trapping HMI in aqueous solutions (see figure 1).

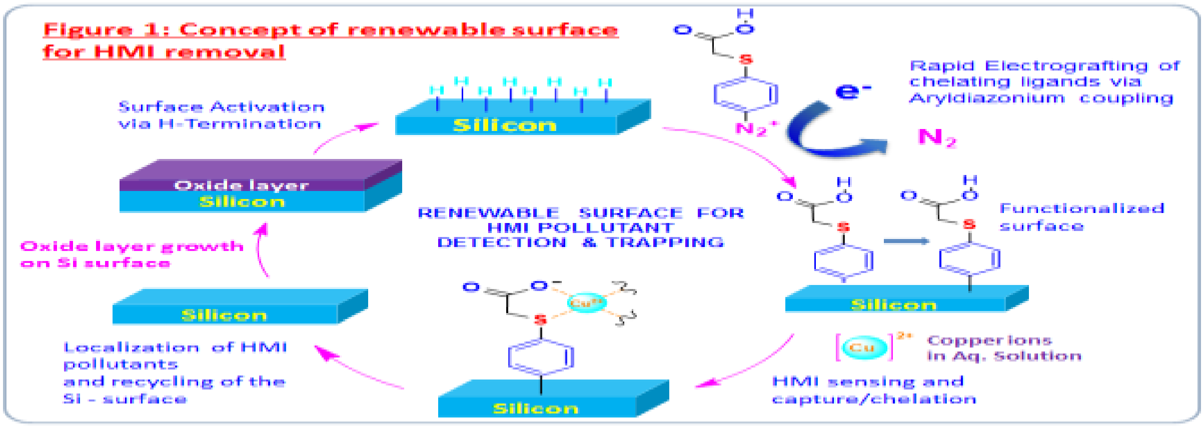
Figure 1: Concept of renewable surface for HMI removal

Infrared spectroscopy confirmed successful surface functionalization by the carboxymethylthio ligand groups. Raman spectroscopy results show that the modified surface is capable of binding Cu ions via chelation mechanisms. X-ray photoelectron spectroscopy also corroborates existence of Cu ions chelated by the carboxymethylthio ligands. A careful washing with acid of the resulting metal-organic complex on the surface followed by surface re-oxidation would provide a breakthrough towards developing a renewable and economical HMI chelating surface for environmental protection.

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Re-examining the influence of a hydrogen termination together with an adsorbate layer from the atmosphere on the characteristics of the subsurface hole gas

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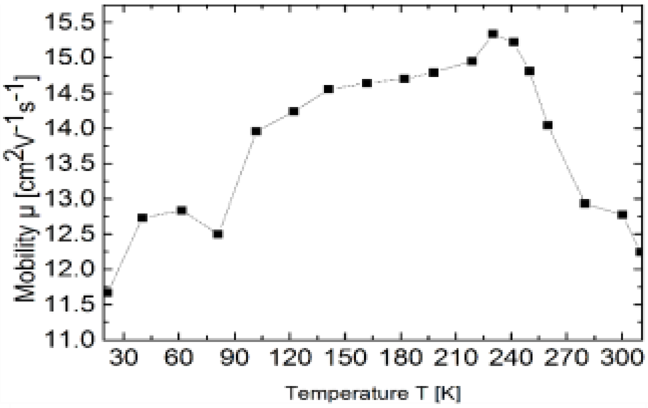

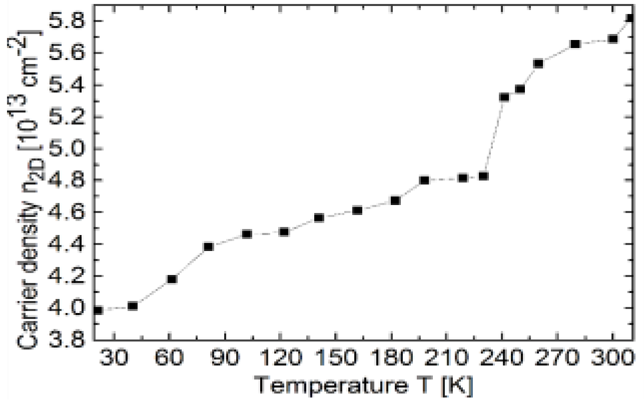

The control of surface conductivity of single crystal CVD diamond by terminating the surface with hydrogen is an useful instrument for manipulating the charge states of shallow nitrogen vacancy centers (NV). These color centers in diamond are practical single photon emitters due to RT operation and are candidates for applications in quantum computing, quantum information technologies and are sensitive magnet field and temperature sensors.

These NV centers were created by ion implantation and a heating step in ultra high vacuum in a depth of 9 nm. For a spatially located implantation a robust surface conductivity is necessary which can be realized by high temperature implantation or by using a hydrogen adsorption induced surface conductivity. For that it is necessary to get a better control of the terminating process by RF plasma to minimize plasma etching on the surface. We have produced a two dimensional hole gas on CVD-grown diamond through an hydrogen plasma with varying parameters and the adsorbtion of water at atmosphere. The established hole gas is characterized with I-V characteristic and with temperature dependent hall experiments. The hall experiments revealed a p-type conductivity with a charge carrier density of $6 \cdot 10^{13}$ cm^{-2} (see lower figure) and mobility of 12 cm^2 V/Vs (see upper figure) at room temperature. The temperature is varied in the range from 20 K up to 310 K, showing a maximum of mobility of 15.5 cm^2 V/Vs at 230 K. The behavior is more characteristic for 3D-hole gas than for the 2D-gas as is usually assumed up to now. Also, we used the van der Pauw method for in situ measuring the temperature dependence of the surface conductivity by heating the diamond in vacuum between 500 K up to 1100 K. In addition to the plasma termination a “mild” termination by activated hydrogen with hot filament in UHV is also tested. Additionally, XPS measurements of the surface revealed the influence of oxygen adsorbates in addition to the H-termination on the mobility and the carrier density on the surface.

Investigating the band structure of phosphorus delta-layers in Si(001)

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The confinement of two-dimensional layers of dopants within semiconductors to form two dimensional electrons gases (2DEGs) has been of considerable scientific interest for some decades. In recent years, that interest has been further heightened by the possibility of exploiting 2DEGs in quantum information processing (QIP) devices [1]. Recent advances in the ability to fabricate and then laterally confine phosphorus (P) dopant 2DEGs in silicon [2], using the technique of hydrogen resist lithography, have led to their use as nanoscale leads and electrodes in devices such as single electron transistors [3]. Consequently, the need to develop a full understanding of their electronic structure has become paramount. Furthermore, it is possible to vary the density of the dopants in a Pin-Si delta-layer by several orders of magnitude, opening up the possibility to study fundamental physics such as the metal- insulator transition and spin-valley physics in the prototypical disordered Hubbard system of reduced dimensionality, where the on-site Hubbard interactions are due to the Coulomb repulsion on the P donor atoms.
Preliminary ARPES experiments were performed on P delta-layer samples in order to investigate the density dependant band structure of the P 2DEG state. We will describe our initial findings and the implications they suggest for future measurements.

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Ab-initio Investigation of Photocatalytic Water Splitting on LiNbO3

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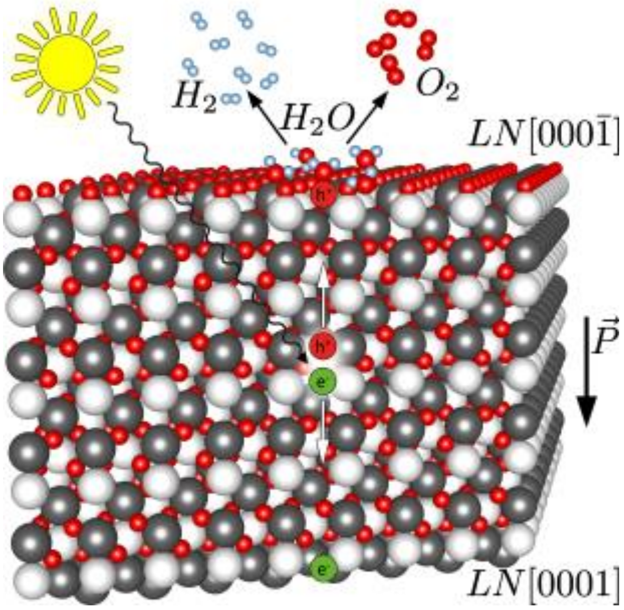

Photocatalytic water splitting for hydrogen production offers a way of clean, low-cost and environmentally friendly production of hydrogen by solar energy. Besides titanium dioxide also ferroelectric lithium niobate has been studied as possible photocatalyst in this context [1]. The internal polarization in this material is expected to lead to a long lifetime of photo-induced carriers as well as reaction athways that involve both the positively and negatively charged surface. The oxidation and reduction half reactions take place spatially separated, which makes the recombination of the products unlikely. In the present work the water splitting at LiNbO3 Z-Cut surfaces is studied within density functional theory (DFT). Thereby the approach of Nørskov et al. [2] for estimating the free energy profile of the oxygen evolution and the hydrogen evolution reactions is followed. Saddle points in the potential energy hypersurface are determined using the nudged elastic band method [3] and constrained DFT is used to model the excited configurations. We find, that the workfunction change upon H2O adsorption, and therefore the molecule-to-substrate charge transport, depends sensitively on the surface termination. The dependence of the latter on the polarization orientation leads to different reactions on the positive and negative surface, respectively.

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Adsorption on water-functionalized Si(001)-(2x1) surfaces

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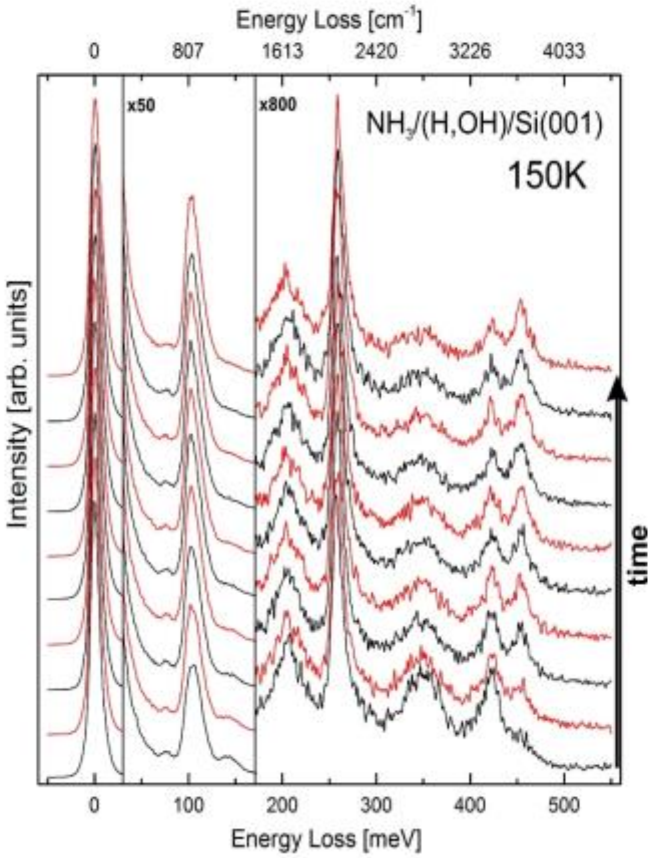
The functionalization of the Si(001)-(2x1) surface by direct deposition of organic molecules has become an interesting topic for research as this way the surface reactivity can specifically tuned to facilitate specific applications in the formation of organic/inorganic semiconductor hybrid structures. Here, a main problem is the large variety of possible adsorption geometries on the Si-surface leading to very inhomogeneously bound molecule layers. A possible solution to this problem is the use of an intermediate water layer enabling a better control of the adsorption processes due the reduction of possible adsorption sites and geometries. Surface bound hydroxyl-groups offer special bonding sites. To investigate the binding properties on those silanol-groups (Si-OH)) and to examine the chemical reactivity we studied the adsorption of propionic acid (CH_3CH_2COOH) at room temperature and ammonia (NH_3) in the temperature range between 100K and 300K as examples of strong and weak interactions, respectively, on a water reacted Si(001)-(2x1) surface using high resolution electron energy loss spectroscopy (HREELS) and photoemission spectroscopy.



For propionic acid the comparison of HREEL-spectra of H_2O and D_2O reacted Si-surfaces shows that the molecule reacts with the surface silanols forming a surface bound ester and the elimination a water molecule.

NH_3 acts as a Lewis base towards surface silanols. Self-limited adsorption on the-silanols in a proton-acceptor geometry (ammonia giving its lone pair to Si-OH) is found below 140K. Taking temperature dependent spectra (see figure), the adsorption and desorption kinetics were quantitatively determined and an activation energy for desorption of 0.41eV was found. In addition, there are indications for the growth of a small amount of dissociated ammonia on remaining isolated dangling bonds of the water covered surface.

Effective narrow ladder model for a correlated wire on a semiconducting substrate

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An effective narrow ladder model (NLM) is used to describe a correlated atomic wire on a semiconducting substrate such as Au/Ge(001), Pt/Ge(001) and Bi/InSb(001). This NLM has been derived by taking only a limited number of legs after exactly mapping a 3-dimensional wire-substrate model onto a 2-dimensional ladder model in which the first leg represents the wire and the rest represents the substrate. The applicability of the NLM as a good approximation to capture the electron-electron correlation effects is discussed using density matrix renormalization group and quantum Monte Carlo simulations for wires represented by spinless fermion as well as Hubbard models. This approach allows us to investigate the role of the substrate in the occurrence and the properties of Luttinger liquids in atomic wires[1].

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Electron Interference in Ballistic Graphene Nanoconstrictions

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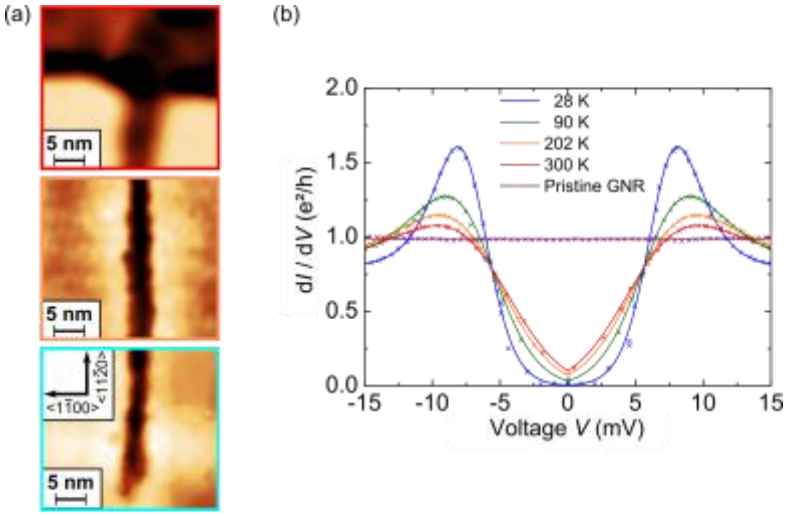
Graphene nanoconstrictions (GNCs) are a central building block of future carbon electronic devices. However, the synthesis of constrictions with well-defined edges is challenging.

Here, we use the tip of a scanning tunneling microscope (STM) for the local etching of graphene, which allows to define GNCs with variable dimensions of down to 1 nm (see Fig. 1 (a)). The GNCs are etched into fully ballistic graphene nanoribbons hosted on the sidewalls of SiC mesa structures [1]. Due to the highly precise etching technique as well as the exceptional electronic quality of the graphene (e.g. mean free path > 10 μm), this system is ideal to study coherent transport phenomena. Therefore, the transport characteristics of constrictions with various dimensions are recorded by means of a variable temperature 4-tip-STM.



Electron interference at the abrupt graphene interfaces gives rise to characteristic conductance peaks and transport gaps which are shown in Fig. 1 (b). Their appearance is described by a tight-binding and recursive Green's function approach which especially highlights the robustness of the resonances features against temperature as well as disorder [2].

Fig. 1. a) STM images of the top, center and bottom part of the cut etched into a sidewall graphene nanoribbon. b) Differential conductance across a GNC with length L = 6 nm and width W = 2 nm for temperatures between T = 28 K and 300 K

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SPA-LEED investigations of quasi one dimensional Dysprosiumsilicide structures on Si(001)

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The investigation of rare earth (RE) metal induced nanowires (NW) on silicon is of particular interest since their quasi one dimensional (1D) structures and the consequential electronic properties are distinctively different from structures of higher dimensionality. Recently, a new class of Si(001) supported quasi-1D systems based on RE silicides (RESi) has attracted attention [1]. Here, RESi submonolayers form a large variety of different superstructures on Si substrates and some of these superstructures have large anisotropic quasi-1D structures. Here, the (2x4) and the (2x7) superstructures [2,3] are of special interest since the latter acts as wetting layer for the formation of NWs if more RE metals are deposited on the Si(001) surface. In addition, further RE deposition leads to the formation of NW bundles as well. This effect has been attributed to strain induced effects due to different 'bulk' structures RESi and Si.

In this work, Dy was deposited on flash annealed Si(001) samples by means of molecular beam epitaxy at elevated temperatures and examined by spot profile analysis low energy electron diffraction(SPA-LEED) as a function of the Dy coverage and the sample temperature. (2×4)- and (2×7)-reconstructions are observed at lower coverages. While the (2x4)-superstructure is well ordered (cf. Fig. 1(a)), the (2x7)-reconstruction shows linear disorder as indicated by streaks appearing in the diffraction pattern (cf. Fig. 1(b)). The formation of these structures appears to be temperature-dependent. A bundling of the NWs can be observed at sample temperatures of 500°C and higher coverages due to the formation of streaks governing the diffraction pattern (cf. Fig. 1(c)). In addition, mean domain sizes were determined from diffraction peak analysis in order to derive the optimal growth parameters for the NWs.

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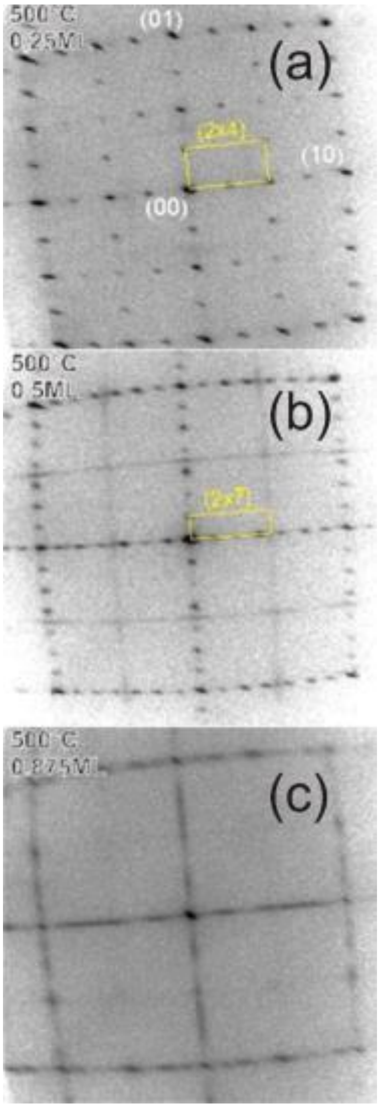

Fig. 1. Diffraction pattern of different (quasi) 1D structures observed after depositing Dy on Si(001) at 500°C. (a) (2x4), (b) (2x7), (c) streaks due to nanowires.

Au/Si(775) atomic scale nanowires:
Structural, electronic, magnetic, and optical properties

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Atomic-scale Au nanowires attached to Si(hhk) substrates have found considerable interest in recent years, because they offer, at least in principle, the possibility to study physical realization of phenomena predicted theoretically for one-dimensional model systems. The Au/Si(775) surface is one of the model systems recently discussed in this context [1]. In particular it was noted that its spin structure deviates considerably from the predictions made for the structurally related Au/Si(553) surface [2]. Here we present a thorough computational analysis of a large number of structural candidates for Au/Si(775). It comprises total energies obtained from density functional theory in conjunction with calculated band structures, spin densities, simulated scanning tunneling microscopy images and surface optical anisotropies. The spectroscopic signatures are compared with experimental data. Interestingly, we find the energetically most favored models to show spin polarized surface states, similar to the case of Si(553)-Au or Si(557)-Au.

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Transport in atomic wires

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Atomic wires on surfaces are prototype 1D systems for studying fundamental aspects, e.g. charge density waves (CDW) or dimensional crossover from a Fermi to a Luttinger liquid behavior. Among others, Au-induced wire structures on Si(hhk) substrates attract a lot of attention because of their quasi-1D metallic structures with a pronounced magnetic order, which mimics a 2D quantum spin liquid state [1]. We present a systematic study on the transport properties of these self-assembled chains of gold atoms on vicinal Si(hhk) surfaces via a multi-tip STM/SEM system in combination with SPALEED.

The characteristics of the Si(553)-Au and Si(557)-Au surfaces were carefully analyzed during in-situ adsorption of molecular oxygen. In combination with recent DFT calculations, we discuss the transport in terms of the different structural building blocks (Au chains, Si-adatom chain, Si edge) found for the Au/Si(hhk) systems [2]. It will be shown, that the origin for the metallic surface bands along the wires are of different origin. Therefore, while the Si(553)-Au surface turns out to be rather immune against oxidation, the Si(557)-Au surface reveals a strong decrease of the conductance due to complete destruction of the Si-adatom ordering along the chains.

In addition, we investigated in detail the surface structure and transport properties of Si(553)-Au as a function of temperature. As seen by electron diffraction, the chains revealed x2 and x3 reconstructions at low temperature, which are associated with ordering along the Au- and Si-step edge atoms, respectively. While the x2 periodicity persists upon annealing, the x3 periodicity of the Si-honeycomb chain structures undergoes an order-disorder transition at T_C=100K. The analysis of the transport data reveals a residual conductivity along the wires below T_C. This shows that the phase transition of the x3 reconstructions comes not along with the formation of a charge density wave, in contrast to previous reports [3, 4].

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Ginzburg-Landau-Langevin and Su-Schrieffer-Heeger theories for the phase transition of In/Si(111)

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We investigate the dynamics of colletive excitations in Peierls insulators using the Ginzburg-Landau-Langevin (GLL) theory for quasi-one-dimensional charge-density-wave systems. This formalism allows us to study the vibrations and the non-equilibrium dynamics of the amplitude modes (lattice distortion and density modulation) which are involved in a Peierls transition. We include no phase mode but amplitude modes for the commensurate Peierls system. We generalize the Peierls theory to include a metastable uniform phase. First goal is to determine the phonon spectrum seen in Raman spectroscopy [1]. Second goal is the generalization of the GLL theory for systems with several Peierls modes. Finally, we calculate parameters for the GLL theory from the microscopic Su-Schrieffer-Heeger (SSH) model in the grand canonical formalism and from firstprinciples simulations [2].

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Density functional theory investigation of rare earth silicide nanowires

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Quasi one-dimensional electron systems are both of fundamental interest because of their unusual physical properties as well as potentially interesting for devices on nanometer scale. In this respect, rare earth (RE) silicide nanowires on silicon (001)-surfaces are of special interest, because 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 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 electronic properties, we have investigated different wire models from first-principles within density functional theory (DFT). Thereby erbium is chosen as a prototypical trivalent rare earth ion, its 4f-electrons treated as frozen states in the atomic core.

All wire models base 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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Time-resolved bond strengths evolution during surface phase transitions calculated from *first principles*

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The In-Si(111)(8x2)/(4x1) nanowire array is an intensively investigated, prototypical example for a quasi-one-dimensional system which features a Peierls instability-driven phase transition, see, e.g. Refs. [1-3]. Experimentally it has been shown that the insulating (8x2) phase undergoes a phase transition towards the metallic (4x1) phase upon optical excitation far below the critical temperature [4]. Here we rationalize this finding by means of ab-initio total-energy and electronic-structure calculations including a detailed bonding analysis. For that purpose we implemented and applied a numerically very efficient Crystal Orbital Hamilton Population (COHP) scheme [5]. In conjunction with ab initio molecular dynamics (AIMD) on excited-state potential energy surfaces we are thus able to monitor the evolution of the surface bond strengths on the Femtosecond time scale. The computationally predicted ultrafast surface structure changes are in excellent agreement with recent time-resolved electron diffraction data from the Horn-von Hoegen group in Duisburg.

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Modification of plasmons in metal-induced atomic wires

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Metallic quasi-one dimensional wires on regularly stepped Si surfaces are heralding potential to investigate exotic quantum phenomena in low dimensional physics, such as quasi-1D collective electron excitations and their crossover to 2D. They may also serve as a basis for future atomic-scale devices. Thereupon, the tunability of plasmonic excitations in the metallic nanowires is of particular interest. The collective electronic behavior undergoes a dramatic change when the geometry is restricted to quasi-1D and electrons in such systems are strongly correlated. Depending on the misorientation against high symmetry directions, regular arrays of straight steps and narrow terraces of well-defined width are generated, while the geometry of steps and metal concentrations allow the formation of self-assembled atomic wires with the regular arrangement. Although, the high reactivity of these systems makes it difficult to change and control of internal properties of ultimate wires. We show that chemical modification not of the wires, but of the more reactive environment triggers a proximity effect that stabilizes and modifies the properties of 1D atomic chains.

Here we illustrate the effect of O_2 and H_2 adsorption on the electronic properties of arrays of single [Si(557)-Au] and double chains of gold [Si(553)-Au] by a study of plasmonic excitations. The plasmonic excitations were investigated via EELS (electron energy loss spectroscopy) combined with SPA-LEED (spot profile analysis-low energy electron diffraction) that provides both high energy and momentum resolution. All measurements were carried out at room temperature under UHV conditions. Dispersion for both systems are only seen along the wires, as expected for a quasi-1D system, and the losses approach zero at small $k_\parallel$, the typical feature of low dimensional plasmons. However, the dispersion curves turn out to be sensitive not only to the local electron density but also to further structural elements such as terrace width, terrace separation and also to adsorbates.

Theoretical results show that oxygen and hydrogen atoms bind preferably not to the Au chains directly but to adjacent Si-honeycomb chains (Si-HC) and Si-adatom rows (The latter exist only in Si(557)-Au). The Si-HC turns out to be mostly responsible for the plasmonic changes. While atomic H reduces the plasmon frequency on Si(553)-Au, as predicted theoretically, adsorbed oxygen leaves it unchanged, whereas a frequency increase is found to be induced by oxygen in Si(557)-Au. Comparing the oxygen results on Si(553)-Au and Si(557)-Au, both the structural motifs (double vs. single chain), as well as electronic distributions across the terraces play a role. These effects still need further detailed consideration in order to separate them clearly.

A New Theoretical Insight Into ZnO NWs Memristive Behavior

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Traditionally the working principle of electrochemical metallization resistive switching devices has been explained in terms of metallic filament formation. Contact metal ions dissolve into an insulating oxide, drift toward the counter electrode and start forming a filament that eventually would connect the two metal contacts turning the device from a high resistance state (HRS) to a low resistance state (LRS).

However, some studies on a ZnO nanowire device showed that LRS might be achieved even without formation of a continuous filament. This rises up questions about the applicability of the conventional theory to nanowire-based devices.

By means of Density Functional Theory simulations, we propose an alternative switching mechanism that involves metal adatoms migrating at the NW surface. Contact atoms rather than forming a filament, spread on the surface. Adatoms, which are extracted from the electrode, are the species that most of all contribute to conduction. Density of states calculations show that adatoms locally dope the surface of the NW creating a surface conductive channel on the NW external shell. Adatom distribution (and therefore the resistance state of the device) is tuned by the external voltage that easily move them back and forth once the electric field intensity exceeds the diffusion barrier. This model predicts switching occurrence even for low densities of contact ions in accordance with the large dimensions of the NW employed in the experimental device.

Hybrid Transfer Method for waveguide structure solar cell

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Abstract

Solar cells provide a renewable and clean energy by converting the sunlight to electricity and it is rapidly considered as an alternative source to the conventional sources. A new waveguide solar cell structure containing 4 layers, the first layer is Air, the second is Aluminum oxynitride (AlONE), the third is Fe-InGaAsP, and the last layer is Silicon( ) is a Substrate, has been investigated in order to improve the light transmission through the considered structure. Light hybrid modes which includes both the transverse electric field and transverse magnetic field of light have been taken into account. Both TE and TM light polarizations through an anti-reflection coating structure have been extracted from the Hybrid Transfer Matrix Method. Hybrid Transfer Matrix Method (TMM) has been implemented to investigate the efficiency of waveguide solar containing semiconductor materials. The Transfer Matrix Method (TMM) which depends on analytical and mathematical bases has been implemented. The transmitted, reflected and absorbed spectra versus the operating wavelength for various of physical parameters as the layers thickness and the type of materials and the incidence angles have been computed numerically. The simulations have been carried out by using the MAPLE software. The effect of substrate silicon layer has been illustrated, analyzed and discussed. This work has shown excellent results for high transmission of the incident waves for certain frequency bands. Hence, the studied structure would be promising to be utilized in the field of solar cells..

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Analysis of the electronic and atomic structure of Pb/Si(557) by polarization dependent two-photon photoemission

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The local structure of atomic wires Pb/Si(557) is determined (i) by the macroscopic quasi one dimensional symmetry imposed by the vicinal cut substrate and (ii) local arrangement of Pb atoms on the Si terraces. We analyze the electronic structure by angle-resolved two-photon photoemission (2PPE) as a function of light polarization and find a dichroism in the 2PPE intensity for opposite electron momenta along the terraces k_x and $-k_x$. Considering earlier work [1] on Pb/Si(111) which concluded on the coexistence of the H3 and T4 symmetry in the $\sqrt{3} \times \sqrt{3}$ reconstruction, the observed polarization dependent dichroism suggests a combination of three and six fold symmetry of the Pb arrangement on Si(557) in agreement with a compressed structure along the Si terrace.

Funding by the DFG through FOR 1700 is gratefully acknowledged.

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Structural, electronic and magnetic characterization of Fe3O4/SiO2/Si heterostructures

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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. Jonker et al reported electrical spin injection into Si from a ferromagnetic Fe contact across an Al2O3 tunnel barrier at low temperature [1]. Later on, Jeon et al reported similar effects at room temperature using crystalline MgO as tunnel barrier [2]. The use of SiO2 as a tunnel 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 Fe3O4 on Si/SiO2 substrates by PLD, with thicknesses ranging between few nm to 80 nm, in order to determine the applicability of FM-semiconductor heterostructures using SiO2 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 Fe3O4 single phase character without silicate formation, ferromagnetism at room temperature, well-defined metal to insulator transition, high quality interfaces and low tunnel barrier thicknesses.

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Morphology-induced phonon spectra of CdSe/CdS nanoplatelets

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Two-dimensional 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, along with bare NPLs (*i.e.* consisting of only single compound, CdSe, CdS, or CdTe) are gaining increasing interest with respect to their fundamental properties and exploring new areas of application. Here they represent interesting materials for studying the elemental excitations under strong confinement along one dimension [2].

We applied Raman and infrared spectroscopy to investigate the phonon spectra and electron-phonon coupling in bare CdSe and CdS NPLs, as well as in core/shell and core-crown CdSe/CdS NPLs [3]. Compared to bare NPLs, core-shell NPLs show a larger number of features in fundamental and multi-phonon Raman scattering spectral range. The Raman spectrum changes dramatically when tuning the resonant laser excitation energy E_{exc} within the absorption range of NPLs and changes even more when switching the excitation to off-resonant conditions. The spectral lineshape in the case of core/shell NPLs is highly sensitive to the shell thickness, while the spectra of the core-crown NPLs more resemble the sum of spectra of the isolated CdSe and CdS particles, and are similar to spherical morphologies studied earlier [4]. This behaviour can be explained by mutual influence of the core and shell in NPLs with the formation of coupled and combined phonon modes. In the core-crown structure, due to the relatively small interface area, the CdSe and CdS modes preserve more independent behaviour, with only interface modes forming overtones with core phonons.

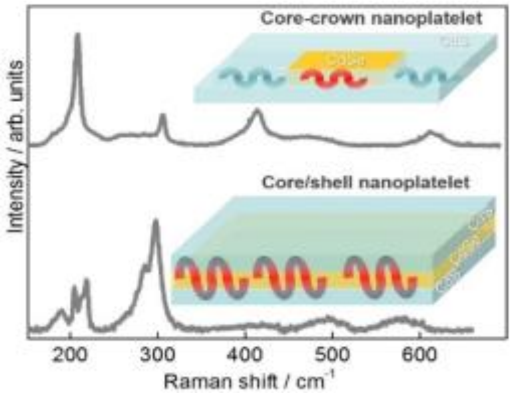

Fig. 1. Representative resonant Raman spectra of two types of CdSe/CdS NPL morphologies shown in the insets.

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Characterization of buried metal/GaN interfaces

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GaN plays a major role in the development of new devices, such as ultraviolet photodetectors, hydrogen sulfide gas sensors [1] and next-generation power devices.[2] However, the interaction of the chemical species and defect states at the metal/GaN interface is rather complicated. For example, Pt and Ni are typical metals used for Schottky contacts, while Ti is regularly used for Ohmic contacts on GaN. After deposition, the metal/GaN stack is usually annealed during a sintering process but resulting Ohmic contacts and Schottky barrier heights at the interface are found to be highly dependent on annealing temperature,[3] are not very stable upon extended heating,[4,5] and are not very reproducible.[6] As one of the most fundamental GaN contacts, this issue requires close inspection.

To reveal the chemical and electronic structure at the buried metal/GaN interface, we deposited Pt, Ni and Ti on c-plane n-type GaN substrates and investigated the samples with synchrotron-based hard x-ray photoemission spectroscopy (HAXPES) at SPring-8 beamline BL15XU. The high information depth of the HAXPES setup (up to about 30 nm) allowed us to analyze the interface of samples with relatively thick metal cover layers. We compare samples as-deposited and after annealing to 350°C or 500°C in N_2 atmosphere. Substrate core levels show distinct energy shifts upon annealing, which can be correlated to the changing Schottky barrier heights - determined with I-V and C-V measurements.

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Surface Raman spectroscopy and first-principles calculations of the vibrational modes of the Au-(√3x√3)/Si(111) reconstruction

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(Sub)monolayer coverage of metal atoms adsorbed on a semiconductor surface may lead to particular reconstructions with specific electronic properties and characteristic vibrational modes. Optical spectroscopy methods are powerful tools for the investigation of these reconstructions: while reflectance anisotropy spectroscopy gives information on the surface morphology and band structure, surface Raman spectroscopy can be employed to study the vibrational modes. Together with first-principles calculations, a comprehensive understanding of the surface vibration dynamics can be obtained and a microscopic model of the surface termination can be established.

For the Au/Si(111) system, surface reconstructions with (5x2) and (√3x√3) periodicity have been observed. Recently, the occurrence of specific Raman modes, which replace the formerly detected eigenvibrations of the clean Si(111)-(7x7) surface [1], was demonstrated for the (5x2) reconstruction [2]. In this work we focus on the (√3x√3) reconstruction of the Au/Si(111) surface, for which the atomic positions are under debate. Four different models were proposed: twisted-trimer (TT), conjugate honeycomb-chained-trimer (CHCT), honeycomb-chained-trimer (HCT), and H_3 missing-top-layer (H_3-MTL) [3,4].

In situ Raman spectra were recorded for different polarization configurations at 300 K and ≈ 20 K. Several signatures exclusive of the Au-induced (√3x√3) reconstruction appear in the Raman spectra, including Peaks at 30 cm^{-1}, 73 cm^{-1}, and a group of peaks around 115 cm^{-1}. Further peaks of minor intensity are found at higher wavenumbers. All the observed peaks vanish with ageing of the samples.

Density functional theory has been employed to investigate the relative stability of the atomic terminations discussed in the literature, and to model their vibrational properties. Thereby, phonon eigenfrequencies and eigenvectors at the Γ point were calculated within the frozen-phonon approximation and classified according to their symmetry. Several surface localized modes of A_1 and E symmetry are found that are well suited to explain the measured Raman data. Combining experimental and theoretical results, we propose a first assignment of specific eigenvectors to the measured Raman peaks.

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Magnetic and Structural Investigations of Ferromagnetic Nanostructures 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 spininjectors. To fabricate well-defined quantum devices, a site-selective spin injection process (in contrast to a large-area approach) is vital. Therefore, spin-injector materials which form selfassembled nanostructures and are compatible with semiconductor substrates are of interest. In this contribution we present growth studies of different potential spin-injector materials on GaAs substrates. Due to their predicted half-metallicity, compatibility with semiconductor substrates and high bulk Curie temperatures MnSb, Fe3Si and CrSb have been chosen as materials for this study. The grown nanoclusters are characterized by STM, LEED, in situ MOKE and SQUID measurements. The influence of different growth parameters on the formation of nanoclusters and their properties such as size, shape, density and magnetic behavior is investigated. Superparamagnetic behavior is found for two of the three materials.

For the application in quantum devices, the spin-injecting nanoclusters have to be spatially oupled to the underlying functional layers, such as semiconductor quantum dots. This can be reached by utilizing the inherent strain induced by the underlying semiconductor QDs as referred nucleation sites for the nanocluster formation. As a preparational step, structural properties, such as island density and size, have to be matched with the underlying pattern of QDs. To reach an island density in the relatively low density range of typical QD samples, the high mobility of Sb on GaAs at elevated temperature together with a weak tendency for intermixing can be used to form templates of nonmagnetic nanostructures (see fig. 1). In a second deposition step these Sb-islands can be transferred into ferromagnetic MnSb nanostructures.

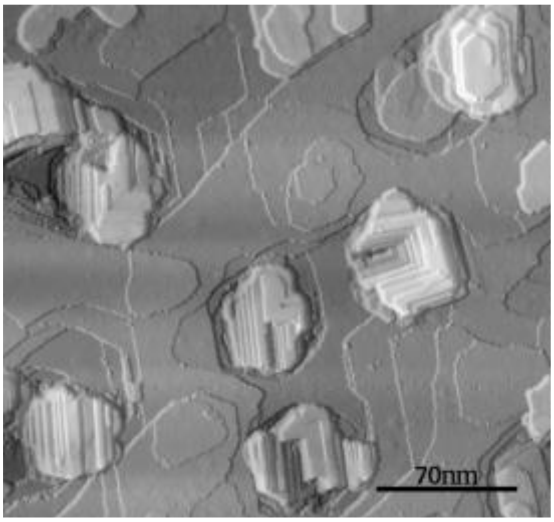

Fig. 1. Example of site-selective growth driven by prestructured substrate. Nucleation of Sb- islands in etch-pits of the GaAs substrate

Structural analysis of Ba_2SiO_4 thin films grown on Si(100)

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Crystalline Ba_2SiO_4 is a very promising candidate as a high-k dielectric. Films grown in a previous study [1] have shown a dielectric constant of 22.8 ± 0.2, band offsets to p-Si(100) of over 2 eV, a high temperature stability up to desorption at around 750 °C and an acceptable leakage current of 3 mA/cm² at -1 V. Unfortunately, these films still feature a high density of interface traps.

The primary cause of this is most likely the growth mode of the silicate films, which were produced by heating the Si(100) substrate during the growth of a BaO film, so that a diffusion of Si from the substrate to the film occurred turning the BaO into Ba_2SiO_4. This process resulted in an atomically rough interface in a geometric and possibly also in a chemical sense. Moreover, only the first 5 nm close to the interface turned out to be crystalline.

This study aims to improve the structural quality of the Ba_2SiO_4 films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion.

The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. To further investigate the crystalline growth, crystal orientation and thickness HRTEM is used.

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Structural Evolution of Hafnium Methacrylate Nanocluster Photoresists following Electron Beam Irradiation from *in situ* IR Spectroscopy

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High absorption metal and main group oxide nanoclusters have recently become the subject of intense investigation due to their potential as alternatives to conventional organic chemically amplified photoresists for negative tone patterning in the extreme ultraviolet (EUV) range. It is believed that the low energy secondary electrons generated from photoionization of the nanoclusters are responsible for the chemistry that occurs following irradiation. Despite their potential, little is known about many aspects of their function as resist materials; in particular, the role of high absorption elements in the absorption/photoionization process, the role of electrons of different energies, the formation of radicals and chemically reactive species and the overall structural changes that occur at each stage of processing. Thus, the precise atomic mechanism underlying solubility switching upon irradiation remains unknown. We have investigated one such class of materials: nanoclusters based on a hafnium oxide core decorated with methacrylic acid ligands (HfMAA) , using a combination of *in situ* infrared (IR) spectroscopy and x-ray photoemission spectroscopy (XPS). Thin films (10-30 nm) of the HfMAA nanoclusters deposited onto SiO_2 from solution are characterized by XPS and IR spectroscopy in conjunction with density functional calculations. The mechanisms of solubility switching following EUV exposure are investigated using irradiation with low energy electrons to emulate the photoexcited carriers generated in the EUV absorption process. Using *in situ* IR spectroscopy, we are able to monitor the structural evolution of the nanoclusters at each stage of processing, beginning from the initial deposition to post application bake (PAB), electron irradiation, post exposure bake (PEB) and development. Monochromatic electron beams with energies ranging from 5 eV up to the typical EUV wavelength of 92 eV enable a correlation between the role of secondary electron energy with chemistry and functional character. In conjunction with XPS analysis, these measurements detail the structural evolution of the films under typical processing conditions, providing insight into the solubility switching mechanism of this emerging class of inorganic photoresists.

Charge transfer dynamics at the buried GaP/Si(001) interface studied by means of time-resolved SHG

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Epitaxially grown GaP on Si(001) is a technologically important and structurally very well characterized model system of a polar/nonpolar semiconductor interface. We have employed time-resolved optical second-harmonic generation (SHG) to investigate the ultrafast charge carrier dynamics at the buried GaP/Si interface.

Upon excitation with a 800-nm 45-fs pump pulse, the isotropic interface SHG signal from a delayed non-collinear probe pulse increases strongly. It exhibits a complex temporal behaviour and eventually decays on a time-scale of more than 30 ps. This observation is surprising as the pump photon energy of 1.55 eV is below the direct band gaps of both GaP (2.8 eV) and Si (3.4 eV) and the optical absorption in both solids is weak. Furthermore, transient signal changes in previous SHG pump-probe experiments were generally much smaller, even in cases when strong pumping saturated optical transitions of the Si surface [1]. Therefore, we propose the existence of interface-specific electronic states at the GaP/Si boundary. Electrons excited by the pump pulse via these interface-states are thus efficiently injected into the conduction band of Si. The resulting transient electric field then gives rise to a SHG response from the Si.

Systematic experiments support this, at first glance, rather speculative interpretation. Thus, we show that the different SHG components of the interface can be distinguished phase-sensitively by utilizing the interference between SHG from GaP bulk and the transients. Wavelength-dependent measurements tuning the energy of the pump pulses between 1.1 eV and 1.8 eV furthermore exhibit a clear resonance of the interface excitation around 1.4 eV.

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Negative Capacitance in Optically Sensitive Metal-Insulator-Semiconductor-Metal Structures on Silicon-on-Insulator

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We report the first demonstration of strong negative capacitance effect under illumination (at 365 nm), in back-to-back combination of a metal-insulator-semiconductor (MIS) and metal-semiconductor (MS) junction planar structures (MISM) with asymmetric Schottky electrodes, on silicon-on-insulator substrates with n-type Si-device layer. The MIS portion of the fabricated MISM structure includes Pt NPs processed at low temperatures by atomic layer deposition in-situ with HfO_2 on thermal-SiO_2 grown on Si-device layer. Filament-type leakage paths induced by voltage-stress of the MIS junction transforms the structure to a varactor and photodetector, whose capacitance is sensitive to frequency also. Illumination of the entire MISM structure, or illumination of only MIS or MS junctions, controls the nature of negative capacitance, where either an almost symmetric double peak or a single-peak behavior can be observed, respectively. The example of measured capacitance-voltage (C-V) characteristics of MISM structure measured under different illumination powers and different frequencies in Fig.1 is shown. Negative capacitance peaks disappear at frequencies higher than 100 kHz. Large tuning ratios of capacitance peaks measured under illumination (power of 2.5 µW) and dark are ~ 105, while voltage sensitivity of capacitance is as high as 15. The behavior of conductance and negative capacitance peaks with illumination and frequency are similar. Negative capacitance is mainly caused by: (a) nonlinear modulation of conductance of the neutral part of the semiconductor; (b) trapping/de-trapping at interfacial states caused by variation in minority carrier density. The existence of interfacial traps, which are enhanced by filamentation process and additional defects due to the embedded Pt NPs, as well as the use of Schottky contacts, are imperative for the appearance of negative capacitance in the MISM structures discussed here. The sensitivity of negative capacitance and conductance to illumination in present device fabricated by standard CMOS technology enables its integration into optoelectronic circuits for different applications.

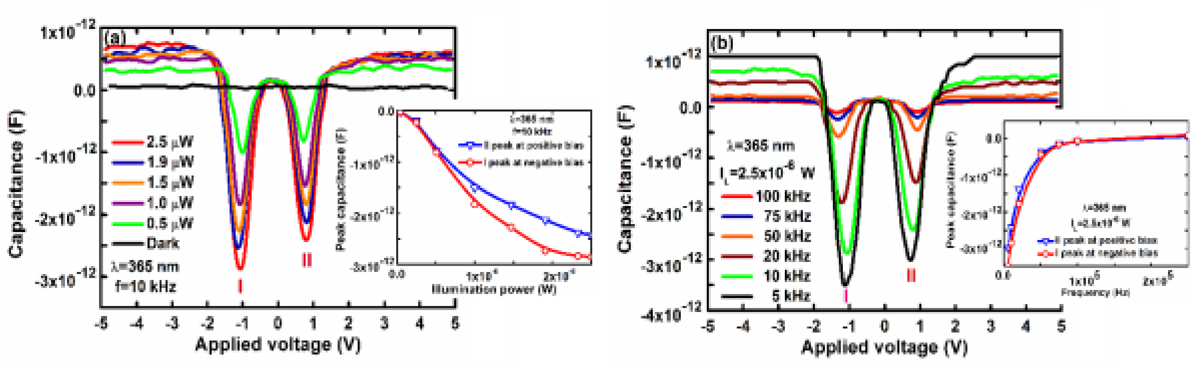

Fig. 1 C-V characteristics of a MISM structure measured (a) at different illumination powers and constant frequency. (b) Different modulation frequencies and a constant illumination power. Insets in (a) and (b), denote respectively illumination power and frequency dependencies of the peak I and II capacitances.

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Photo Sensitive Metal-Insulator-Metal Like Capacitor on Silicon with SrFeO-F Nano Particles Embedded in the Insulator Stack

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We have demonstrated a new type of varactor comprising a metal-insulator-semiconductor (MIS) structure, which incorporates Fe mixed with SrF_2 nanoparticles (NPs) like SrFeO-F, embedded in an insulator stack, between thermal SiO_2 and atomic layer deposited (ALD) HfO_2 sublayers, as seen in Fig. 1(a). This is the consequence of the ALD and rapid thermal annealing processes, which initiate the fluoridation-oxidation and crystallization of the electron-beam gun deposited SrF_2-Fe-SrF_2 sublayers, which was seen in electron energy loss and energy dispersive X-ray spectroscopy measurements. The result is the formation of high-density positive charge sites of the oxygen reduced Fe ions, which, in turn, induce dipole-type traps with electronic polarization. Measured capacitance is bias-independent (see Fig.1 (b)), which resembles the behavior of a metal-insulator-metal (MIM) diode; except that here, the capacitance depends on illumination and exhibits a strong frequency dispersion, as seen in Fig. 1 (c) and (d). Due to large density of traps at the interface, there is significant band bending at Si-interface irrespective of the applied voltage (due to pinning of the fermi level), causing the formation of interfacial inversion layer, playing role of the second electrode. The capacitance is enhanced in the presence of illumination, while capacitance dispersion is rather conventional, reducing with increased frequency. The varactor exhibits extremely low quadratic voltage coefficient. The proposed MIM like capacitor is compatible with standard CMOS technology and can be prepared at relatively low temperatures

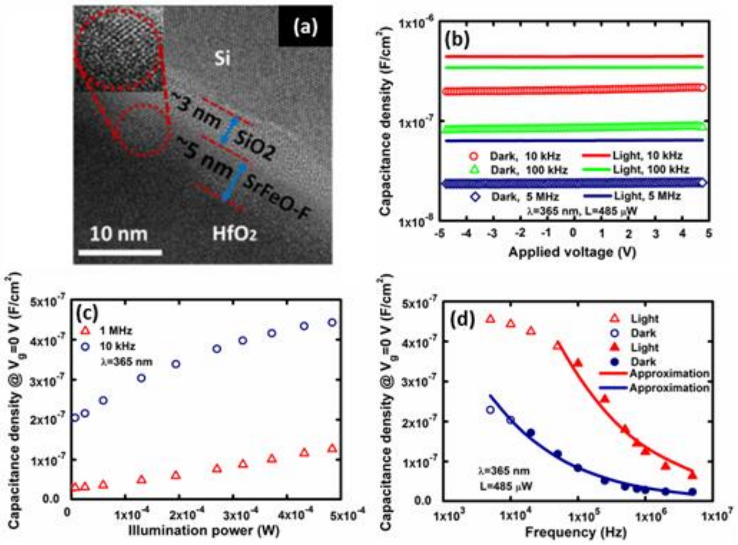

Fig. 1 (a) Cross-section HRTEM micrograph of MIM-like structure with embedded SrF_2-Fe-SrF_2 nano laminates. (b) Capacitance-voltage characteristics of MIM structure measured in dark and illumination regimes at different frequencies. Zero bias capacitance density versus (c) illumination power and (d) frequency. Inset of (a) is the magnified image of the NPs.

Engineering ultra-sharp, ultra-dense doping profiles in silicon: conduction and valence band quantization

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A rather unique branch of the 2D material family are so-called δ-layers, and like their well-known cousins: graphene and layered transition metal dichalcogenides, they too exhibit remarkable quantum properties. δ-layers are ultra-sharp, ultra-dense doping profiles typically achieved in semiconductors. The composition and structure of phosphorus δ-layers in silicon (Si:P δ-layers) have been studied down to the atomic limit by both secondary ion mass spectrometry and scanning tunnelling microscopy, and recently, angle-resolved photoemission spectroscopy has provided direct access to their electronic properties [1]. It is essential that the properties of Si:P δ-layers be understood, particularly in light of the fact, that atomically precise lithography of Si:P δ-layers has led to the fabrication of functioning atomic-scale devices including, the world's narrowest conducting wire [2] and the single-atom transistor [3]; major technological successes towards the development of quantum computers. Confinement of the P dopants to a single atomic plane beneath the Si surface leads to a lowering and discretization of the conduction band (CB) resulting in two parabolic-like states, referred to as 1Γ and 2Γ, dispersing across the Fermi level. We can tune the quantization of CB states by either adjusting the density or profile of the P dopant layer. Confinement of valence band (VB)-derived states between the P dopants and the Si surface additionally leads to quantization, and we can both control and tune the number of these VB quantized states, following a simple-particle-in-a-box model, by simply varying the position of the P dopant layer beneath the Si surface. This case of simultaneous quantization of electron and hole states is atypical of traditional doped semiconductors, and as such these Si:P δ-layers provide new opportunities for not only engineering materials with new properties but radically changing the way in which atomic-scale devices are both designed and fabricated.

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Frequency shifts and Raman signatures at ferroelectric domain interfaces of $LiNbO_3$ and $LiTaO_3$ modeled by first principles

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Periodically poled lithium niobate ($LiNbO_3$, LN) and lithium tantalate ($LiTaO_3$, LT) structures are of particular technological interest as waveguides and SHG structures [1]. The interface between neighboring domains features a large polarization gradient, which causes a modulation of numerous physical properties, e.g. the internal strain, birefringence and Raman cross section [2]. In recent years, several experimental techniques, including Raman spectroscopy [3], have been utilized to image those domain wall structures. In this theoretical work, vibrational properties and Raman signatures of LN and LT in the vicinity of domain walls are studied within a simple empirical model based on atomistic density functional theory (DFT) first principles calculations, which were performed for the ferroelectric and paraelectric bulk phases of LN/LT. Frequency shifts and Raman intensities of E and A_1 modes with respect to a phenomenological reaction coordinate between both phases are in qualitative agreement with the experimental data. In particular, the soft mode behavior of the low frequency A_1-TO_1 mode, a characteristic feature of ferroelectric phase transitions [4], can be reproduced.

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Electronic interaction between CdTe quantum dots and PEDOT:PSS: a photoluminescence quenching study

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The strong and size-dependent photoluminescence (PL) of quantum dots (QDs) is one of the reasons of the high interest in these nanostructures and application in light-emitting diodes, luminescent bio-imaging *etc.* [1]. On the other hand, the monitoring of the photoluminescence (PL) is an efficient and convenient experimental probe for the interaction between the surface of QDs and the environment and forms the basis for sensor applications [2]. Composites of QDs with conjugated polymers were recently reported as being capable of photostimulated charge transfer and separation and such systems are interesting for photovoltaic applications [3,4]. Monitoring the QD PL can be used as a straightforward criterion indicating charge transfer. Here, we report on PL monitoring of CdTe QDs with mean sizes of about 2, 3, 4, and 5 nm by PEDOT:PSS in aqueous solutions. It was found that for reduction of an integrated PL intensity in 100 times, 6 times less amount of polymer is needed in case of 2 nm QDs than for 5 nm QDs. Furthermore, the addition of PEDOT:PSS results in significant bathochromic shift (up to 0.3 eV) of the PL band of CdTe QDs (fig.1). The magnitude of the shifts decreases with increasing QD size and are finally negligible for 5 nm CdTe QDs. The value of the shift is proportional to the amount of PEDOT:PSS and increase during sample storage time. The results obtained indicate the strong and controllable interaction between the QDs and the PEDOT:PSS polymer. The possible mechanisms underlying the observed effects are discussed based on additional information obtained by X-ray and UV photoemission, Raman and IR spectroscopies as well as electron microscopy.

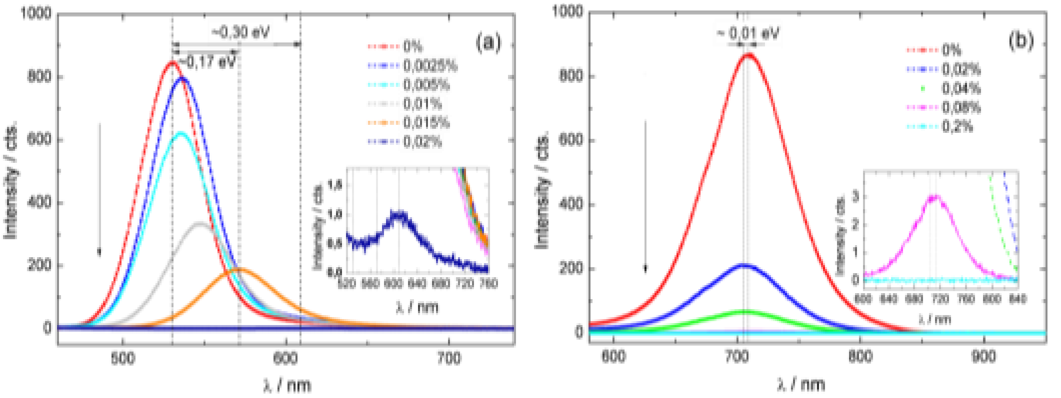

Fig.1.Evolution of the PL spectra of CdTe QDs in water solution with increasing concentration of PEDOT:PSS for 2 nm QDs (a) and 5 nm QDs (b). The insets show the enlarged spectra for (a) 0.02% and (b) 0.08% and 0.2% of PEDOT:PSS in solution.

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Investigation of the effects of different post-annealing conditions on the electrical, structural and optical properties of vanadium oxide thin films

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Vanadium oxide (VOx) thin films are preferred for microelectronic devices, sensors, optoelectronic systems and microelectromechanical systems (MEMS) due to its outstanding properties [1,2]. The electrical properties of VOx thin films are generally related to arameters such as the structural phases (VO2, V2O3, V2O5, V3O7, V6O13, etc.), film thickness and grain size. Between different phases, especially, VO2 is desired due to its extended electrical and optical properties [3,4]. Pulsed DC magnetron sputtering technique is one of the preferred technique to obtain VOx thin films; however, the high deposition or post-annealing temperatures (>400°C) make production of the films with VO2 phase crucial [1, 2, 4-7]. For most of applications, the process temperature must kept as low as possible (<400°C) to make the thin film layer compatible. Therefore, optimization of the post annealing process is one of the popular issue. In this present work, the VOx thin films were grown on Si/SiO2, Si/SiO2/Si3N4 and quartz (x-cut) substrates with 100 nm thickness by using Pulsed DC Magnetron Sputtering technique without introducing substrate heating. After deposition, films were annealed at temperatures below 300 °C under vacuum and pure N2 atmosphere. Prior investigations on structural properties indicate that the as-deposited film has mostly amorphous-polycrystalline structure with grain size ranging from 5-20 nm. The film contains dominantly VO2 phase; however, depending on the post-annealing conditions, besides VO2 phase, other phases such as V2O5, V3O7 and V6O13 were also observed. The high resolution electron microscopy investigations reveal that the crystallinity of the films increases with rising post-annealing time and temperature. On the other hand, pores in nanoscale were also observed. The structural observations make the structure-property correlation interesting, hence, in the present work, the influence of post-annealing conditions on the correlation between structural, electrical and optical properties were discussed and presented.

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Study of the photoinduced hidden state in 1*T*-TaS_2 single crystals doped with selenium by means of time-resolved photoemission spectroscopy

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We study the relaxation dynamics in the strong-excitation regime in the quasi-two-dimensional transition-metal dichalcogenide 1*T*-TaS_2 doped with selenium by means of non-equilibrium time-resolved photoemission spectroscopy (tr-ARPES). In agreement with the preliminary optical pump-probe experiments [1,2] we observe a transition to a new hidden state (H-state) which is inaccessible under normal equilibrium conditions and can only be reached after a quench with a single femtosecond laser pulse at 1.6-4.8 mJ/cm^2 fluence. By means of tr-ARPES we achieve well defined switching to the H-state which manifests itself in the significant quench of the lower Hubbard band (LHB) spectral signature causing a modification of the electronic structure of the system [2]. In addition, a notable change in the coherent phonon spectra plays the role of fingerprint of the achieved switching to the H-state via optical path. This discovery is of great importance not only to the physics of nonequilibrium dynamics of dichalcogenides but should also provoke some interdisciplinary interest in the computer memory device industry.

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Self-Assembled Monolayers of Oriented Dipoles as a Tool for Altering of Semiconductor Interfaces

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Self-assembled monolayers (SAMs) can alter the surface properties of various substrates in a desired way, which represents a highly innovative technological approach. The SAMs of polar organic molecules were successfully used for adjusting the metal work function (see for example [1] or metals and proved useful in constructing various organic thin-film devices. However, the applicability of SAMs is limited by relatively low thermal stabilities of organic molecules – most of them dissosiate already at 200 °C. To make this approach more applicable the used SAMs should endure temperatures up to 400 °C (CMOS process).

In this regard, SAMs of carboranes with exceptionally high thermal stability represent promising candidates [2]. Carboranes ($C_2B_{10}H_{12}$) are compounds composed of carbon, boron, and hydrogen, whose molecular geometry is derived from an icosahedron. Introducing two carbon atoms in the boron cage leads to the formation of high dipole moment in the molecule (4.3 D for *ortho*-carborane isomer). It has been shown that SAMs of the carborane-dipoles can be easily prepared on gold and silver surfaces *via* thiol (SH) functional groups. Silver work-function can be tuned very precisely over a range of 1 eV by using a mixture of oppositely oriented carborane-thiol dipoles [3].

In this work, we investigate: 1) the stability of created SAMs of *ortho*-carborane dipoles on silicon substrate by Kelvin Probe Force Microscopy (KPFM), 2) the effect of different carborane isomers on the substrate work function, and 3) the influence of the SAMs on the interface barrier in 2-layer semiconductor structures.

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Laser-induced transformations in cadmium-doped As_2S_3 films

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Amorphous arsenic sulphide As_2S_3 is a well known semiconductor material extensively studied in view of its photosensitivity and possible applications related mostly to reversible or irreversible photoinduced effects. Doped As_2S_3 glasses and films are much less investigated. The present study of thin (1–2 µm) As_2Se_3:Cd films grown by thermal evaporation was performed using atomic force microscopy (AFM), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and micro-Raman spectroscopy.

As_2S_3 films with a nominal Cd content of 1 to 4% were grown by thermal evaporation on silicate glass and Si substrates. AFM imaging (Agilent AFM 5420) reveals a uniform film surface with a roughness of 0.4–0.9 nm. EDX measurements performed using a Nova NanoSEM microscope with different electron energies (5–30 keV) show that for each sample the content of cadmium rapidly decreases with the probing depth. Still, for each electron energy value a qualitative correlation is observed between the nominal Cd content in the film and its value determined from the EDX spectra.

Micro-Raman measurements performed at 295 K using a Horiba LabRAM spectrometer and a 514.7 nm or a 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 undoped As_2S_3 films with a dominant broad feature near 335 cm^{-1} and a weaker one near 230 cm^{-1} that is a clear evidence of their amorphous structure. Contrary to the undoped As_2S_3, a new sharp peak near 300 cm^{-1} as well as a smaller maximum near 600 cm^{-1} appear for the Cd-doped films with increasing P_{exc}. The onset power density for the appearance of these peaks is lower for higher Cd content while the band positions and intensities depend on the laser power density and wavelength. These new peaks appear within the illumination time of several seconds and do not disappear after the excitation power is lowered again, which suggests that the laser-induced local photostructural changes in the film are quite fast and irreversible. The emerging features can be explained by the formation of CdS nanocrystals in the laser spot area: the corresponding LO and 2LO phonon frequencies for CdSe are 305 and 610 cm^{-1}, respectively. The peak frequencies observed in the As_2S_3:Cd film spectra are slightly lower because of tensile strain experienced by the nanocrystals resulting from the photoplastic effect (a radial mass transfer from the laser spot) in the films. The tensile strain values are determined from the Raman spectra. The geometrical parameters of the pit at the laser spot are examined based on the AFM and SEM data.

Defect-induced strain broadening of the infrared zero-phonon line of the NV$^-$ center in diamond

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The negatively charged nitrogen-vacancy (NV$^-$) center in diamond has attracted numerous research efforts aimed towards its applications in spin-based quantum sensing and quantum computing devices [1-4]. The inhomogeneous broadening of the optical and spin resonances of NV$^-$ centers is a key limitation of many of these applications. It is currently believed that this broadening is principally caused by the inhomogeneous strain and electromagnetic fields generated by random microscopic distributions of defects, such as the substitutional nitrogen center.

Here, we examine the splitting and inhomogeneous broadening of the NV$^-$ center's infrared (IR) zero-phonon line (ZPL). We develop a model for these effects by adapting the strain broadening theory proposed in Ref [5]. We apply this model to interpret observed variations of the IR ZPL shape with temperature and photoexcitation conditions. We identify an anomalous temperature dependent broadening mechanism and that defects other than the substitutional nitrogen center significantly contribute to strain broadening. The former conclusion suggests the presence of a strong Jahn-Teller effect in the center's singlet levels and the latter indicates that major sources of broadening are yet to be identified. These conclusions have important implications for the understanding of the center and the engineering of diamond quantum devices. Finally, we propose that the IR ZPL has the potential to be used as a sensitive spectroscopic tool for defect micro-/nanoscale tomography.

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STM visualization of surface and subsurface atomic structure of Gd_3Si_5/Si(111) using clean and oxygen-terminated tungsten tips

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The role of the tip electronic structure and tunneling gap resistance in atomically resolved scanning tunneling microscopy (STM) experiments has been investigated in numerous works [1-3]. It has been demonstrated that tip-sample interaction can modify the electron orbital structure of the tip and surface atoms at tunneling gaps comparable with interatomic distances in solids [4,5]. This can lead to changes of the spatial resolution during distance-dependent STM experiments and, in certain cases, to direct visualization of the electron orbital structure of the front tip atom at very small gaps [4]. Here we report results of the distance- and voltage-dependent STM studies conducted on the well-ordered Gd_3Si_5/Si(111) system using clean and oxygen-terminated tungsten probes. The experiments show that atomic-resolution STM images measured with both tips reflect the atomic structure of buried vacancies down to the fifth subsurface layer at a metallic surface, which is hardly accessible by other experimental techniques. In order to confirm this picture, we have performed the total energy density functional theory calculations and STM image simulations that go beyond the Tersoff-Hamann approach. The simulations support the unusual STM depth sensitivity for this system. Analysis of the STM data obtained with clean and oxygen-terminated tungsten probes shows that atomic resolution can be achieved at larger gap resistances (larger tip-sample distances) in the latter case. The experimentally observed atomic corrugations are approximately two times larger in the case of the functionalized tungsten probe. The STM image simulations suggest that the difference in atomic corrugations is related to different relaxations of the tungsten and oxygen tip atoms interacting with the surface silicon atoms. At small gaps the oxygen-terminated tungsten probes produce asymmetric features with depressions above the surface silicon atoms, which can reflect the electronic structure of the tip rather than electronic structure of the surface.

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Feasibility study on topological quantum field effect transistor of silicene, germanene and stanene nanoribbons with edge hydrogen termination

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Silicene, germanene and stanene are novel two-dimensional honeycomb allotropes of silicon, germanium and tin atoms, respectively. They are counterpart of graphene and show exotic electronic and optical properties [1,2] . Their band gaps can be controlled by external fields since they have sp^3-like (low buckled) geometry different from graphene [3,4]. In addition, it is expected that quantum spin Hall states can be observed at experimentally possible temperature due to larger spin orbit coupling than graphene [5,6]. From the two features, a topological quantum transistor of zigzag silicene nanoribbons has been proposed within the single-orbital tight-binding model [7]. We showed that the dispersion of the edge states of zigzag silicene nanoribbons with the edge hydrogen termination is nonlinear due to the multi-orbital effects [8], different from the single-orbital tight-binding model. The edge states appear in the bulk band gap. Therefore, understanding the behavior of the edge states is prerequisite for the realization of the topological quantum transistor.

In this study, we investigate the dispersion of edge states of silicene, germanene and stanene with hydrogenated zigzag edges in the presence of vertical electric fields, by using the multi-orbital tight-binding model. In general, the ground state of the zigzag nanoribbons is the anti-ferromagnetic state. In order to obtain the correct ground state within the tight-binding model, we implemented the mean field approximation in our multi-orbital tight-binding model. We found that the bulk band gap of the zigzag nanoribbons decreases as the strength of the electric fields increases. However, there are the edge states in the band gap except for stanene. In our presentation, we discuss whether a topological quantum transistor can be realized by zigzag silicene nanoribbons or not, together with the results of germanene and stanene.

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Transport of Top and Bottom Surface States in Ultra-Thin Bismuth Films

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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 and alloy formation [1], 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 magnetic field dependent transport.

Beside the top surface state an additional state at the Si/Bi interface has been proposed [4], that is also spin polarized by the Rashba effect. For symmetry reason the spin polarization in this bottom surface state is opposite with respect to the top surface.

Angle dependent magneto-conductance measurements for various thicknesses were performed. In particular, the parallel field magneto-conductance, with a magnetic field in the plane of the sample surface, either parallel ($G_{par.}$) or perpendicular ($G_{perp.}$) to the current direction, grants additional information about the scattering processes between the top and bottom surface [2]. The magneto conductance is found to be highly anisotropic. For all thicknesses $G_{par.}(B)$ is dominated by weak-anti-localization (WAL) and as the film thickness decreases the coupling strength between the interfaces increase. This may give rise to an additional state in the bandgap [3]. The transport $G_{perp.}(B)$ is dominated by weak-localization (WL) that is most likely due to direct backscattering from +**k** states in the top surface to –**k** states in the bottom surface. A transition from WL to WAL for the thinnest film (20 BL) has been observed, revealing the coupling induced reduction of the spin polarization as also observed in SRARPES measurements [4].

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Scanning Laue X-ray Nanodiffraction for Microstructural Imaging and Its Applications for Detecting Crystal Structure of 2D Materials

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The X-ray Nanodiffraction Beamline (XND) is one of the phase-I projects for Taiwan Photon Source (TPS). The end-station called “FORMOSA (FOcus x-Ray for MicrOStructure Analysis)” is dedicated to use the focusing white/mono-beam Laue diffraction for structural analysis. For instance, users could obtain the 2D and 3D distribution of crystal phases, orientation, residual strain, stress and dislocations for materials in a complex form without distorting the sample during measurement. The current spatial resolution is better than 90 x 90 nm at lateral direction and 50 nm for depth. Furthermore, this end-station also provided many complementary tools. Tetra-probe stages could deploy several scanning probes to collect optical, electrical, surface properties with tens of nanometer resolution of specimens; the x-ray fluorescence detector provides elemental information and the cryo-stage integrated with heater for temperature dependence experiments. Particularly, it is also the first time in synchrotron history to integrate an online scanning electron microscopy (SEM) as a navigator. With spatial resolution down to 4 nm, it is able to find out the interest region with tiny structure on samples and also arrange the position for different probes. This end-station can function either in vacuum or ambient environments depending on the user’s demands. In summary, XND beamline and FORMOSA end-station will provide not only 2D/3D-XRD but also XRF, XAS,

XEOL/CL, SPM and SEM information for diverse research programs. This work will show you some recent results for crystal structure determination of 2D materials, and ist related thin film system on silicon substrate and sapphire.

Direct measurement of the excitonic energy gap of Ta_2NiSe_5 single crystal

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The excitonic insulator (EI) was first proposed in 1967 theoretically[1], but only few materials have been suggested to be EIs[2-5]. Mostly, the indirect experimental evidences of the EI state such as transport measurements or renormalization of band dispersions have been reported. The energy gap of an EI candidate, Ta_2NiSe_5, in a low temperature phase was recently measured for the first time through the optical spectroscopy, and attempt to control the EI state was reported with pressure and substitution of Se or Te for S. However, neither of the direct measurement of single-electron energy spectra nor atomically local control of the EI state has been achieved yet. We carried out scanning tunneling microscopy / spectroscopy (STM/S) measurements at room temperature and 78 K, as well as theoretical model calculations to investigate the electronic structure of Ta_2NiSe_5. Ta_2NiSe_5 shows metal-insulator phase transition in our STM/S experiments, with an energy gap of 550 meV at 78 K. Furthermore, the orbital characters at the valence and conduction band edges are inverted at low temperature. This indicates a strong hybridization between Ta and Ni bands, one of important evidences of the EI state. The two-band and three-band model calculations support our experimental results, the energy gap opening with band inversions. These results reveal that the EI mechanism in Ta_2NiSe_5 is close to the Bardeen-Cooper-Schrieffer (BCS) condensation of cooper pairs. We dosed K on Ta_2NiSe_5 to manipulate the EI state and found out that K atoms prefer sitting on bright chains of Ta_2NiSe_5. The EI state is robust against the atomic impurities, since in-gap states are measured only at the vicinity of K atoms.

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Optical control of ultrafast currents in the topological surface state of Sb_2Te_3

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We present energy-momentum mapping of the photocurrent in the spin polarized Dirac cone of the topological insulator Sb_2Te_3 by means of time- and angle-resolved two-photon photoemission (2PPE) after optical excitation with ultrashort tunable mid-infrared laser pulses. In previous work we have demonstrated that linear polarized mid-infrared pulses permit the generation of photocurrents with ps-lifetime in the initially unoccupied part of the Dirac cone of Sb_2Te_3 by a direct optical excitation. By observing the decay of the asymmetric population, we can directly investigate the dynamics of the long-lived photocurrent in the time domain [1].

Here we show that the magnitude and direction of this current depends on the azimuthal orientation of the sample and that the current can be coherently controlled by the polarization of the pump light by means of the linear and circular photogalvanic effect [2]. For azimuthal orientations for which no photocurrent is generated by linear polarized pump light, we are able to generate a photocurrent by elliptical polarized light only and fully control its direction and magnitude by varying the light helicity of the mid-infrared light by a l/4-plate (Figure 1).

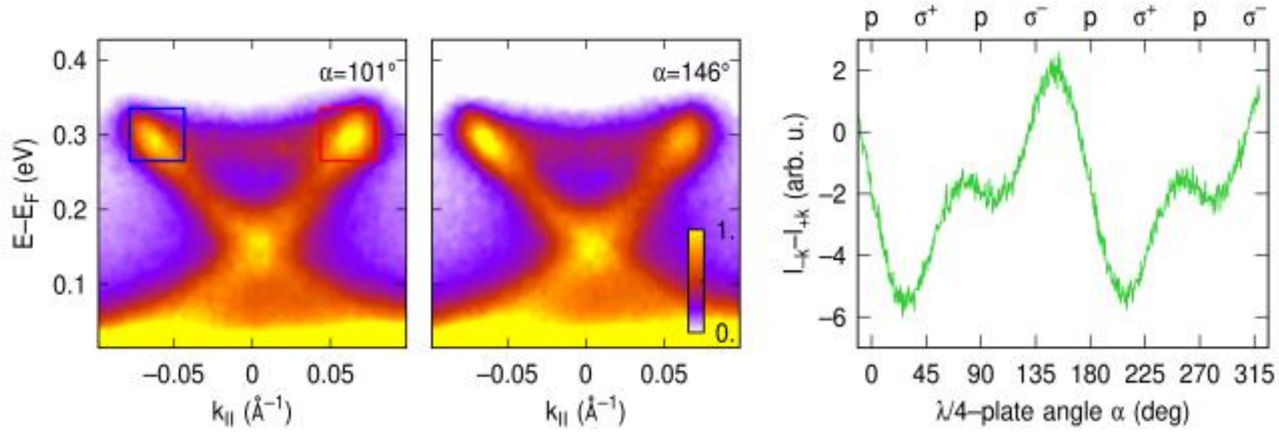

Figure 1: Angle-resolved 2PPE spectra of Sb_2Te_3 for mid-IR pump (hn=0.33 eV) of different helicity.

[1] K. Kuroda *et al.*, Phys. Rev. Lett. **116**, 076801 (2016).

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Scattering of surface state carriers in Bi(111) nanofilms, grown on Si(111) by Pb and Sb adatoms

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The surfaces of semimetallic thin-film systems, such as Bi(111), exhibit strong similarities with topological insulators. They represent a relatively simple, easy to prepare system to study questions related to topological insulators. The quantum size effect makes thin films semiconducting in the bulk at low temperature so that transport properties of epitaxial Bi films are mainly due to surface conductance in the strongly spin-split surface electronic states that cross the Fermi level.

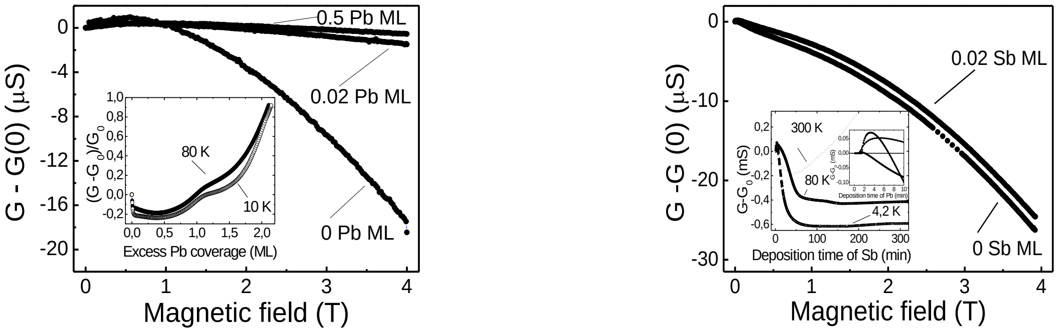

Fig. 1. Change of magneto- and electrical (inserts) conductance of 20BL epitaxial film Bi(111) during adsorption of Pb (left) and Sb (right). G_0 and G(0) is conductance at zero adsorbate coverage and in zero magnetic field.

Our investigation of modifications of surface magneto-conductance by Pb or Sb adsorption on Bi(111)-films, grown epitaxially on Si(111) substrate, complements earlier studies of the effect of impurity scattering by adsorbed atoms with varying magnetic moments and charge transfer between adatoms and surface states [1-4]. Pb adsorption leads to the initial sharp electrical conductance decrease caused by increasing of carrier scattering on adatoms (Fig 1, left). Sb adsorption results in the initial conductance increase (Fig. 1, right) due to charge redistribution between adatoms and surface electronic states, followed by a decrease as a function of Sb concentration, caused by enhanced surface scattering. Comparison of scattering efficiency of different adatoms (Bi, Co, Fe, Tb, Cr, Pb, Sb), as determined by magnetoconductance and Hall resistance measurements demonstrates that Sb adatoms are the weakest scatterers.

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Surface and bulk magnetic gapping in the electronic structure of (V, Fe, Mn) doped BiTeI.

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Magnetic doping of topological insulators (TIs) and Rashba systems characterized by enhanced spin-orbit (SO) coupling and helical spin structure leads to opening of an energy gap at the Dirac point and formation of new exotic topological quantum effects such as Quantum Anomalous Hall effects, topological surface-state magneto-electric effects, giant Kerr and Faraday rotation of polarized light and others and can be used in spintronics for manipulation of spin state and induced magnetization without external magnetic field [1]. Here we study magnetically doped polar semiconductor BiTeI with giant Rashba splitting and time-reversal symmetry breaking. BiTeI by itself has a hexagonal crystal structure and is built up of alternating layers of bismuth, tellurium, and iodine atoms stacked along the hexagonal axis. The continuous stacking order of the layers of the three atomic species breaks the inversion symmetry. Therefore, we study the time reversal symmetry breaking in magnetically doped Rashba semiconductor BiTeI. Similar behavior of the surface states takes place in magnetically doped topological insulators [2,3] the magnetic gap opens at the Dirac point. Spin-orbit interaction in 2DEG with broken inversion symmetry results in the Rashba splitting of the electronic states. Combination of the Rashba and magnetic interaction with superconductivity using proximity effect can lead to topologically non-trivial superconductivity and Majorana fermion mode [4].

BiTeI is characterized by bulk and surface Rashba-like states, and thus below the Curie temperature we expect that the magnetic gap can open in both types of states. Measurements of these systems were made by means of UV-ARPES, during which it has been shown the presence of the gap with no zero density of states in the surface Rashba states with the value of 120 meV. In order to investigate the behavior of bulk states we had carried out the Soft X-ray Photoemission Spectroscopy (SX-ARPES) since this method lets us to probe the electronic states at a depth of 15-20 Å. Thus the different photon energies were used to distinguish bulk and surface states. Using high energy that is sensitive to bulk it is possible to conclude with high accuracy that bulk Rasba states of the sample have no magnetic gap. To distinguish the role of the magnetic moment induced by ferromagnetic dopants, we will use V, Fe and Mn $L_{2,3}$-edge resonant photoemission supported by Circular Dichroism absorption spectroscopy.

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