Physics at the borderline between 1D and 2D

Workshop of the Nanowire Network in Bad Honnef

13-15 February 2013

organized by

FOM-1D, FOR1162, FOR1700

NWO

DFG Deutsche Forschungsgemeinschaft

Content

Publisher:

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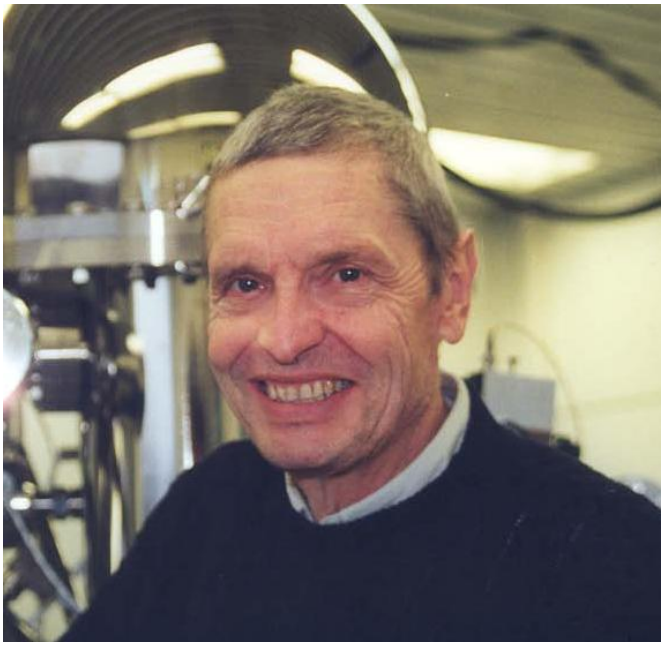
Cover picture: Physikzentrum Bad Honnef (PBH), taken from Web

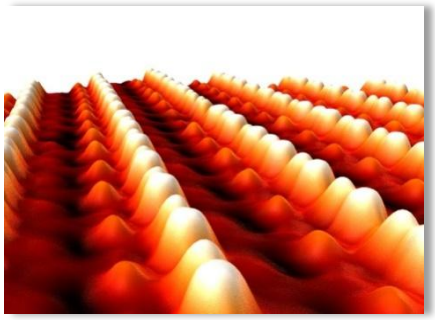


Stefan Hüfner

1935 – 2013

The present workshop on *"Physics at the borderline between 1D and 2D"* follows the long-standing tradition of the annual *Aschermittwochs-Rundgespräche,* also known as *Hüfner-Seminars*, since for decades they have been organized by Stefan Hüfner. As spokesperson of the DFG Priority Program on *"High-Energy Spectroscopy"* he initiated this workshop series in 1985 as an important forum for scientific exchange in the field of surface science, dedicated especially to applications of the then new technique of photoelectron spectroscopy and related methods. Shaped by Stefan´s personal style and the homely atmosphere of the *Physikzentrum*, the meetings soon developed their unique character with ample time for thorough and passionate discussions, as we have come to know and love them. Stefan fortunately managed to keep up the meetings beyond the end of the Priority Program, always finding interesting topics within and beyond surface science (and the necessary funding!). And so they continued to be held every year, always starting on an Ash Wednesday, and always taking place in the *Physikzentrum Bad Honnef*, with the late-night discussions in the Bürgerkeller being just as important (if not even more…) as the scientific program during the day.

Sadly, we just learned that Stefan Hüfner has passed away on January 17, 2013. He will be dearly missed. We wish to dedicate this year´s *Hüfner-Seminar* to his memory.



About FOM-1D

The main objective of this FOM programme is to realize, study, understand and ultimately tailor the physical properties of one-dimensional (electron) systems.
The physics of one-dimensional electronic systems is fundamentally determined by interactions. Unlike in Fermi liquid systems, where interactions simply lead to the smooth deformation of electrons into electron-like quasiparticles, interactions in 1D induce remarkably strong correlations. These strong correlations translate into the disappearance of the electron as a fundamental unit, and its replacement by charge and spin collective modes with distinct experimental signatures. These counterintuitive properties should be universal to 1D systems.
From an experimental point of view, truly 1D electron systems are much harder to realize than their 2D and 3D counterparts, which is the main reason why this field of research is still relatively unexplored. On the other hand, theoretical predictions based on the Luttinger liquid paradigm have historically been limited to the low-energy sector, and have thus proved to be difficult to measure even in the few experimentally realized examples. The majority of studies on 1D electron gases have been performed using cleaved-edge overgrowth substrates and carbon nanotubes. These types of systems are ideal to study the power-law correlations of the transport properties, however they are less suitable for studying non-Fermi liquid phenomena in the proximity of defects or impurities. The latter is especially important since many signatures of non-Fermi liquid behaviour develop and prominently show up in the vicinity of defects and/or impurities. One of the main aims of this proposal to controllably study the effect of defects and impurities on the properties of 1D systems. This requires (1) atomistic control over the material which only recently became possible and (2) experimental techniques with a spatial resolution down to the atomic scale.
This programme will provide a concerted team effort between experiment and theory, combining complementary methods for the generation of 1D electron systems with a battery of nano-manipulation and imaging techniques operating in real and reciprocal space, as well as various other characterization techniques, and geared towards making contact with recent theoretical breakthroughs in our understanding and capabilities to compute measurable observables of 1D electron systems.
Some key data:

- 11 principal investigators, 8 PhD students and 1 postdoc
- 5 universities (Leiden, Eindhoven, Delft, Amsterdam and Twente)
- 7 experimental projects, 2 theoretical projects
- Speaker: Harold Zandvliet
- Started: mid 2010

About FOR1162

The Research Unit FOR1162 is a DFG-funded research initiative of several experimental and theoretical groups at the University of Würzburg, targeted at the collaborative investigation of electronic correlation effects and emergent phenomena in nanostructured surfaces and interfaces. The central aim is a microscopic understanding of competing interactions in systems with reduced dimensionality and their effect on the macroscopic electronic and magnetic properties. Surfaces and interfaces are particularly well suited for this purpose as they allow precise preparation and manipulation down to atomic length scales, thereby facilitating active control and tunability of relevant interaction parameters. Systems of interest include self-organized 1D and 2D metal adsorbate structures on semiconductor and metal surfaces, 4*f* metal surface alloys, and conducting interfaces in transition metal oxide heterostructures. Depending on their specific properties they represent versatile model systems for the study of prototypical correlation phenomena such as the breakdown of Fermi liquid physics in 1D, the occurrence of Mott-Hubbard physics in frustrated 2D lattice geometries, or the emergence of heavy-fermion behavior in 2D Kondo systems. Additionally, the interplay of electronic correlations and strong spin-orbit coupling which can be induced by incorporating high-*Z* elements into the surface/interface systems are investigated. These scientific questions are tackled with a wide range of (mostly spectroscopic) surface science techniques in close cooperation with advanced quantum-mechanical many-body theory. The combination of different but complementary methods available within the Research Unit represents a powerful approach in the pursuit of its objectives.

Some key data:

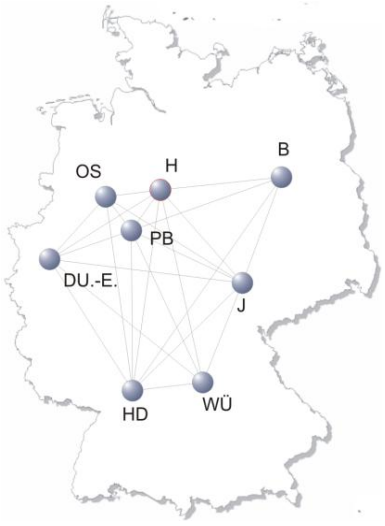
- Local Research Unit, 11 principal investigators
- 6 experimental and 3 theoretical projects
- Speaker: Ralph Claessen
- Webpage: http://www.physik.uniwuerzburg.de/for_1162/
- Second period of funding: Spring 2013

About FOR1700

The central task of the research unit FOR1700, funded by the DFG, is the exploration and identification of physical scenarios with one-dimensional properties under explicit consideration of 2D and 3D coupling, their control and their manipulation.
Ideal one-dimensional (1D) electronic systems have peculiar properties, such as quantization of conductance, charge-density waves (CDWs), and Luttinger liquid behavior, a variety of instabilities with a wealth of associated phase transitions. This highly interesting field is still largely unexplored both from the experimental and the theoretical side. Metallic nanowires are prototype 1D systems. FOR1700 will concentrate on these systems, and will explicitly consider them on well defined Si and Ge surfaces with cross-sectional widths of only a few atomic lattice constants. They will be grown by self-assembly with noble metals (Pt, Au), Pb, In and with silicides of rare earth elements and transition metals. Using both high symmetry planes and appropriate vicinal Si and Ge surfaces we will investigate systematically the intriguing question of coupling between wires, coupling to the underlying substrate and to the 3D embedding material. We plan to explore the consequences of these interactions with respect to intrinsic instabilities (e.g. formation of charge density waves) and potential functionalities. Our investigations will comprise both studies of ground state as well as of excited state properties in order to get information about electron-electron and electron-phonon coupling. Therefore, the structure and phase transitions in the wires and their electronic structure as a function of temperature and of wire density will be correlated with electronic transport, single particle and collective (plasmonic) excitations as well as with their dynamics. In order to explore this field with its great variety of physical phenomena successfully and in reasonable depth, a close collaboration between experimental and theoretical groups is envisaged as well as the combination of various experimental methods.

Some key data:

- 17 principal investigators from 11 institutions at 8 locations
- 5 experimental projects, 2 theoretical projects
- Speakers: Herbert Pfnür, Christoph Tegenkamp
- Webpage: www.atomicwires.de
- Started: 1 December 2012



Program Overview

Wednesday, 13 February 2013

From 13:00		Arrival Physikzentrum Bad Honnef
15:00	Welcome	Presentation of FOM-1D, FOR1162, FOR1700
15:40	Hanno Weitering -invited-	Polaronic transport and current blockades in epitaxial silicide nanowires and nanowire arrays.
16:30-17:10		Coffee break
17:10 – 17:50	Eric Jeckelmann	Physical scales of one-dimensional phenomena in real systems
17:50 -18:30	Christoph Tegenkamp	Spin density waves in strongly interacting Pb wires on Si(557)
18:30 – 19:00	Julian Aulbach	Low-temperature superstructure of Au-induced atom chains on high-index silicon surfaces
From 19:00		Buffet-style dinner

Thursday,	**14 February 2013**	
7:45		Breakfast
8:50-9:30	Raoul van Gastel	Strain- and electronically stabilized low dimensional systems studied by LEEM
9:30-10:10	Martin Hohenadler	Interaction-range effects in one dimension
10:10-10:50	Friedhelm Bechstedt	"Optical excitations in 1D and 2D systems from first principles".
10:50-11:20		Coffee break /Posters
11:20-12:10	Shuji Hasegawa -invited-	Topological and superconducting surface states
12:10-12:50	Jörg Schäfer	Three-Dimensional Spin Texture of the Fermi Surface of a Strongly Spin Orbit Coupled Interface
12:50-14:30		Lunch
14:30-15:10	Sven Rogge	From dopant atoms to solid state molecules
15:10-15:50	Jan van Ruitenbeek	Experimental approach towards three-terminal single-molecule electron transport
15:50-16:20		Coffee break /Posters
16:20-17:10	Walt de Heer -invited-	Structured epitaxial graphene
17:10-17:40	Lydia El-Kareh	"Quasi-particle interference mapping of electronic states in clean and Bi-covered fcc (111) surfaces"
17:40-19:00	Poster session	
From 19:15		Buffet-style conference dinner

Friday **15 February 2013**

7:45		Breakfast
8:40-9:30	Leonid Glazman -invited-	Effect of charge disorder on the conduction along the edge of a two-dimensional topological insulator
9:30-10:10	Annemarie Pucci	Surface Optical Spectroscopy of Metal Nanostructures
10:10-10:50	Martin Wolf	Ultrafast Dynamics of CDW systems probed by time-resolved ARPES
10:50-11:20		Coffee break /Posters
11:20-12:00	Achim Schöll	Photoelectron spectroscopy of organic layers and interfaces: from orbital mapping to Kondo resonances
12:00-12:30	Gang Li	Competing phases of the Hubbard model on a triangular lattice - insights from the entropy
12:30		Lunch / End of Workshop

Coffee breaks & Meals

- Breakfast is provided in the **Physikzentrum** (starts at 7:45 in the "Speisesaal") and the **Hotel Seminaris.**

- Lunch is served in the Physikzentrum Bad Honnef im "Speisesaal" .
  Vegatarians will be asked in advance.

- During the breaks coffee, tea and biscuits will be served in front of the lecture hall (Wilhelm und Else Heraeus-Hörsaal).

- Buffet-style dinner is served in the "Bürgerstube" located in the basement of the Physikzentrum.

Internet access in the Physikzentrum

To access the wireless LAN service in the Physikzentrum please connect to the access point named “PBH” and use the following settings:

- Infrastructure mode (“access point”)
- No authentication
- WPA-PSK encryption with the following key (HEX):
- 011235813 “the first 8 Fibonacci numbers (not digits)”
- Automatic TCP/IP configuration (DHCP)

Venue

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Please note:
Absolutely NO SMOKING in the entire house; there are smoke detectors in every room which are directly connected with the fire station.

Talks

Invited talk Wednesday 15:40

Polaronic transport and current blockades in epitaxial silicide nanowires and nanowire arrays

Hanno Weitering

Department of Physics and Astronomy, University of Tennessee

Abstract

Quantum transport is at the heart of nanoscience and marries a fundamental law of nature, quantum mechanics, with applied electrical engineering and emerging materials technologies. Ultimately, nanoscale electronic devices will contain networks of wires whose cross sections will be so small as to represent quasi one-dimensional conductors with novel transport properties. Among the many intriguing nanowire systems synthesized in recent years, epitaxial metal-silicide nanowires may be the most practical electrical interconnects because of their low resistivity, stable Schottky barriers, and compatibility with the scalable silicon platform. In this talk, I will discuss some of the idiosyncrasies of quasi one-dimensional electron systems and present a detailed analysis of the electronic structure and electrical transport properties of some of the thinnest epitaxial YSi2 nanowires, measured using a four-tip scanning tunneling microscope. Conduction through individual nanowires follows an inverse Arrhenius behavior indicative of thermally-assisted tunneling of small polarons between defect centers. A scaling analysis of the I-V data produces microscopic parameters such as the phonon frequency, polaron shift, and the number of trapping centers; the latter showing a remarkable consistency between STM and transport results. Quantitative analysis of individual wire resistances, probe resistances, and negative differential resistances of nanowire networks furthermore indicates significant electronic interwire coupling below 150 K. The long-range coupling mechanism involves the dielectric polarization of the substrate, inducing current blockades in neighboring conduction channels. This study demonstrates the feasibility of nanoscale circuit analysis using four-point probe measurements, but also points towards the need for utmost control of atomic-scale defects in the electrical and materials engineering of novel nano-architectures.

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Physical scales of one-dimensional phenomena in real systems

Eric Jeckelmann

Institut für Theoretische Physik, Leibniz Universität Hannover, Germany

Abstract

Theory predicts that one-dimensional systems feature unusual properties, such as Peierls transitions and Luttinger liquids, which set them apart from ordinary three-dimensional matter. Physicists have been looking for these effects in strongly-anisotropic three-dimensional solids for several decades. It has become evident that the behavior of quasi-one-dimensional systems changes smoothly from one-dimensional to two- or three-dimensional as a function of the energy, temperature, length, etc..scales which are probed. Unluckily, these scales depend sensitively on the details of the system considered. Thus we expect one-dimensional physics to be observable in experiments at specific but mostly unpredictable scales only. In this talk I will give a brief introduction to and overview of this problem.

Spin density waves in strongly interacting Pb wires on Si(557)

C. Tegenkamp[1], D. Lükermann[1], H. Pfnür[1], B. Slomski[2,3], G. Landolt[2,3] ,H. Dil[2,3]

[1] *Institut für Festkörperphysik, ATMOS, Leibniz Universität Hannover, Germany*
[2] *Physik-Institut, Universität Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland*
[3] *Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland*

Abstract

The growth of atomic wires on semi-conducting templates by self assembly is a promising approach to address fundamental aspects of low dimensional physics, e.g. charge density waves (In/Si(111) [1]) and Luttinger liquids (Au/Ge(100) [2]) under explicit control of the atomic structure. Recently, even spin-orbit coupling (SOC) in such strongly anisotropic systems came into the focus of research as this may cause magnetically ordered states like it is proposed, e.g for Au/Si(553) [3]. Pb/Si(557) is a further impressive example of how semiconducting surfaces can be functionalized by adsorption of a physical monolayer. The mutual interplay between superlattice structures, band filling factors and spin orbit coupling results in a highly correlated electronic spin- and charge-state found for an array of atomic Pb wires grown on Si(557). By means of spin- and angle-resolved photoemission spectroscopy the spin texture close to the Fermi surface was found to be alternating and equidistant, thus Fermi nesting occurs in between bands with the same spin helicity giving rise to spin-polarized charge density waves in the direction across the wires. An out-of-phase superposition of both Rashba-channels is manifested by an extraordinary large Rashba-splitting of $\Delta k_0 = 0.2\text{Å}^{-1} = g/2$, where g is a reciprocal lattice vector defined by the interwire distance, and fits into the model of spin density waves in antiferromagnetically ordered chain structures [4].

The transport properties of the nested phase have been studied systematically as a function of temperature, excess Pb coverage and external magnetic field. Above 78K, the system undergoes a refacetting transition and the system switches into a 2d- transport regime. Excess Pb coverage up to 0.1ML decorates predominantly even-numbered step sites indicating a strong electron-electron correlation across steps. Strong anisotropic magneto-transport was found for Pb-wetting layers close to completion of the physical monolayer caused by an enhanced elastic scattering rate in the direction perpendicular to the step direction. Furthermore, anti-localization is found for all monolayer structures due to strong spin-orbit coupling which is effectively switched off around 1.3 ML pointing towards spin-polarized transport in the nested regime [5].

[1] T. Tanikawa et.al. Phys. Rev. Lett. 93, 016801 (2004).
[2] C. Blumenstein et.al. Nat. Phys. 7, 776 (2011).
[3] S.C. Erwin, F. J. Himpsel, Nature Communications 1, 58 (2010).
[4] C. Tegenkamp, D. Lükermann, H. Pfnür, B. Slomski, G. Landolt H. Dil, Phys. Rev. Lett. **109**, 266401 (2012).
[5] D. Lükermann et.al. PRB **81**, 125429 (2010).

Low-temperature superstructure of Au-induced atom chains on high-index silicon surfaces

J. Aulbach[1], J. Schäfer[1], S. C. Erwin[2], S. Meyer[1], L. Dudy[1], B. Slomski[3], G. Landolt[3], H. Dil[3], R. Claessen[1]

[1]*Physikalisches Institut, Universität Würzburg, Germany,*
[2]*Naval Research Laboratory, Washington DC, USA,*
[3]*Paul Scherrer Institut, Villigen, Switzerland*

Abstract

Self-organized nanowires on high-index semiconductor substrates provide a versatile playground to scrutinize the low-temperature ground state of quasi-one-dimensional systems, such as a charge density wave (CDW) or a Tomonaga-Luttinger liquid. Here we report on Au nanowires on Si(553), where a structural model from density functional theory (DFT) [1] suggests strong spin-orbit coupling for the Au chains. Intriguingly, also antiferromagnetic spin order is proposed for the silicon structure along the terrace edges.

Scanning tunneling microscopy images of Au/Si(553) are found to be in astounding agreement with the structural model [1], including its periodicities. Moreover, tunneling spectroscopy measurements at low temperature indicate the absence of an energy gap. This does not support the picture of two coexisting CDWs, contrary to previous perception. Instead, the local density of states displays a distinctive structure which matches the spin-polarized Si step-edge state predicted by DFT. Finally, we briefly address the spin-orbit coupling in the Au bands using spin- and angle-resolved photoemission, providing direct evidence for a spin-splitting.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010).

Strain- and electronically stabilized low dimensional systems studied by LEEM

Raoul van Gastel[1], Tjeerd R.J. Bollmann[1], Daniel Kaminski[2], Harold J.W. Zandvliet[1], Elias Vlieg[2], and Bene Poelsema[1]

[1]*Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands*
[2]*Solid State Chemistry, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands*

Abstract

The self-organization of two-dimensional films into distinct patterns can result from a variety of physical forces. Patterns stabilized by elastic, electrostatic or magnetic forces are commonly found in literature. Low energy electron microscopy (LEEM) directly visualizes the patterns and allows both qualitative and quantitative information to be obtained from LEEM images and their spectroscopic variants.

In this presentation I will highlight the unusual behavior of Bi adlayers on Cu(111) and Ni(111) surfaces. On Ni(111) quantum well states exist between the vacuum interface of the film and that formed by a Bi wetting layer [1]. Surprisingly, films of different thickness yield different structures. The origin of this electronically induced variation of the atomic structure is found to reside in the variation of the Fermi wavelength for different film thicknesses and structures.

On Cu(111) on the other hand, elastic forces between different phases formed by the Bi dominate, and a strain-stabilized pattern is observed [2]. The morphology of the pattern undergoes a distinct transition at a temperature of 680 K. Using the diffracted intensity in LEEM images, the nature of this transition could be traced back to an order-disorder transition that occurs in one of the two Bi phases that constitute the self-assembled domain pattern.

[1] T.R.J. Bollmann, R. van Gastel, H.J.W. Zandvliet, and B. Poelsema,
Physical Review Letters 107 (2011), 176102.
[2] R. van Gastel, D. Kaminski, E. Vlieg, and B. Poelsema,
Physical Review Letters 109 (2012), 195501.

Interaction-range effects in one dimension

Martin Hohenadler

Institut für Theoretische Physik, Universität Würzburg, Germany

Abstract

The continuous-time quantum Monte Carlo method is used to explore the effects of the electron-electron and electron-phonon interaction range in one dimension. Nonlocal electron-electron interactions play a role in a number of experimental systems, including quantum wires and self-organized gold chains. We calculate the Luttinger liquid interaction parameter as a function of interaction range, and study the impact of the latter on signatures of spin-charge separation. The role of nonlocal electron-phonon coupling has been studied, for example, in the context of superconductivity. Here we obtain the phase diagram at half filling, which supports metallic, Peierls insulating and phase separated regions.

Optical excitations in 1D and 2D systems from first principles

Friedhelm Bechstedt

IFTO and ETSF, Friedrich-Schiller-Universität Jena, Germany

Abstract

The basic ideas of the many-body treatment of excitations and resulting optical properties are illustrated independent of the dimensionality of an electronic system. It represents a three-step procedure toward to find the atomic geometry and to include quasiparticle, excitonic and local-field effects. This procedure is used to investigate many-body effects in the spectra of one- and two-dimensional materials:

(i) The one-dimensional (1D) chains on an In/Si(111) surface show a metal-insulator transition between the 4x1 and 8x2 reconstructions due to a Peierls instability in a triple band system. The relation of interband transitions and surface reflectance anisotropy spectroscopy is discussed.

(ii) In two-dimensional (2D) hydrogenated group-IV crystals silicane and germanane giant electron-hole-pair binding is predicted as a consequence of the reduced screening in two dimensions. The oscillator strength of the exciton bound states is by three orders of magnitude larger than in graphane.

(iii) The infrared absorbance of 2D graphene is nearly independent of frequency and approaches a value determined by the Sommerfeld fine structure constant. We show that this result is conserved for the buckled honeycomb crystals silicene and germanene independent of the gauge of the electromagnetic field. The influence of spin-orbit interaction is also discussed.

Invited talk Thursday 11:20

Topological and superconducting surface states

Shuji HASEGAWA
Department of Physics, School of Science, University of Tokyo, JAPAN

Abstract

Crystals surfaces are a unique platform for many-body physics because of, compared with inside of bulk crystals, much more degrees of freedom in atomic structures, fewer coordinates, low dimensionality, larger fluctuation, broken symmetry, weaker screening, and so on. Phenomena brought about by electron-phonon, electron-electron, spin-orbit couplings at surfaces are sometimes very different from their counterparts in bulk crystals. In my talk, I will show two topics relating surface electronic states, surface-state superconductivity and surface Rasha effect/topological surface states.

Transports of charge as well as spin at crystal surfaces are now intensively studied due to interests of fundamental physics as well as possible applications to devices. Surface electronic states are generally decoupled from the bulk states and therefore intrinsically low-dimensional. Furthermore, space-inversion symmetry is broken down at crystal surfaces. These effects provide rich physics of transport, especially on surfaces of strong electron-phonon-coupling (EPC) and spin-orbit-coupling (SOC) materials.

A Silicon surface covered with a monolayer-regime Indium, Si(111)-R7xR3-In surface superstructure [1], is known to show a large electron-phonon coupling constant [2,3] and exhibit an energy-gap opening below about 3 K in STS, which is assigned to be a superconducting gap [4]. The subsequent research actually showed the zero-resistance on this surface [5]. We have also recently confirmed by resistance measurements with a 'sub-Kelvin micro-four-point probe method in UHV' [6]. This is the first example of 'surface-state superconductors'. The resistance decreases due to fluctuating Cooper pairs above the superconducting transition temperature because of the two-dimensionality. A monolayer Pb-induced surface superstructure, Si(111)-Striped-In commensurate (SIC) phase also showed a SC transition around 1 K. Both superconducting surfaces exhibit much shorter coherence lengths of Cooper pairs than those of bulk indium and Pb. This is due to the 2D nature [7].

The surface-state bands of strong SOC crystals such as Bi and Bi alloys, are known to be spin-split, which is called as Rashba effect [8-11]. Similar effect is observed on a special kind of materials called topological insulators such as BiSb, BiSe, and BiTe alloys. Some of them have spin-split Dirac-cone type surface-state bands. This implies that spin-polarized current will flow at the surfaces of such materials. By using samples of pure Bi [8-11], BiSb [12], BiSe [13,14], and BiTe, I will show that the surface-state bands are really spin-split and the Dirac-cone conductivity is directly measured by in situ microscopic four-point probe method in UHV. An on-going project to detect the spin-polarization of surface current by using magnetic tips in a four-tip STM will be also introduced.

[1] J. W. Park and M. H. Kang, Phys. Rev. Lett. 109, 166102 (2012).
[2] S. H. Uhm and H. W. Yeom, Phys. Rev. B 86, 245408 (2012).
[3] S. Yamazaki, et al., Phys. Rev. Lett. 106, 116802 (2011).
[4] T. Zhang et al., Nature Phys. 6, 104 (2010).
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[6] M. Yamada, T. Hirahara, S. Hasegawa, H. Mizuno, Y. Miyatake, and T. Nagamura, e-J.Surf.Sci. Nanotech. 10, 400 (2012)
[7] M. Yamada, T. Hirahara, S. Hasegawa, Phys. Rev. Lett., submitted.
[8] T. Hirahara, et al., Phys. Rev. Lett. 97, 146803 (2006).
[9] T. Hirahara, et al., Phys. Rev. B 76,153305 (2007).
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[11] T Hirahara, et al., New J. Phys. 10, 083038 (2008).
[12] T .Hirahara, et al., Phys. Rev. B81, 165422 (2010).
[13] Y. Sakamoto, et al., Phys. Rev. B81, 165432 (2010).
[14] T. Hirahara, et al., Phys. Rev. B82, 155309 (2010).

Three-Dimensional Spin Texture of the Fermi Surface of a Strongly Spin-Orbit Coupled Interface

J. Schäfer[1], P. Höpfner[1], A. Fleszar[2], J. H. Dil[3], B. Slomski[3], W. Hanke[2], R. Claessen[1]

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[3]*Paul Scherrer Institut, Villigen, Switzerland*

Abstract

Semiconductor surfaces with metal adatom reconstructions of the (√3 x √3)-type are attracting increasing scientific interest in the last years. This is owed to the rich body of low-dimensional physics encountered therein, which comprises, e.g., highly correlated Mott-Hubbard insulating phases which may give rise to magnetic ordering, as well as two-dimensional superconductivity. Moreover, this metal-semiconductor interface is of high technological interest. Since the space inversion symmetry is broken, a Rashba-type spin-orbit coupling must be expected to lift the spin degeneracy of the metal-induced surface states. A significant spin-splitting in a conducting, two-dimensional electron system at a semiconductor surface would be highly desirable, since it offers the perspective to manipulate spins electronically.

We report on a fully three-dimensional analysis of the spin properties in the metallic surface system Au/Ge(111) based on spin-resolved photoelectron spectroscopy as well as advanced density functional modeling [1]. Surprisingly, and contrary to a conventional Rashba picture, we find that the spin texture exhibits strong out-of-plane spin components, which follow the threefold symmetry of the substrate lattice. Moreover, additional radial spin components are observed in experiment for the first time. Notably, these findings bear close resemblance to theoretical predictions for topological insulators. As we will illustrate in conjunction with model Hamiltonians, these findings reveal an interplay with Dresselhaus-like spin-orbit effects as a result of the crystalline anisotropies. This points at the complexity of the spin-orbit interaction in such real-world systems.

[1] P. Höpfner, J. Schäfer, et al., Phys. Rev. Lett. 108, 186801 (2012), Editors' Suggestion.

From dopant atoms to solid state molecules

Sven Rogge

Centre for Quantum Computation & Communication Technology
School of Physics
The University of New South Wales

Abstract

Dopant atoms have recently been used to demonstrate quantum functionality in solid-state devices. At the same time, it became possible to place dopant atoms with sub-nanometerprecision in 3 dimensions in a silicon device. This atomic-precision dopant engineering allows ultra-scaled devices, building blocks of quantum devices, and potentially artificial molecules in the solid state. Here, we present a study of the simplest possible molecular system in the solid state, a hydrogen atom. We study the bond formation as a function of ion distance. The solid-state environment allows arbitrary distances so it is possible to study configurations that don't occur in nature such as the weakly coupled Heidler-London limit. The transition spectra and quantum-state images agree well with the insight gained from a model of the correlated two-charge state. This represents the first step towards atomically precise chains of atoms in a semiconductor matrix.

Experimental approach towards three-terminal single-molecule electron transport

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Abstract

We consider the problem of electron transport properties of single molecules bridging two metal electrodes. This is a problem of considerable fundamental interest, where we can attempt to connect the large body of knowledge of organic chemistry to the concepts and theories of electron transport in condensed matter systems. The great experimental challenge that one needs to face is bridging the gap in size between the smallest features that can be made by microfabrication, and the size of the molecules to be investigated. One of the most successful approaches to this challenge is by mechanically controllable break junctions, which allow for mechanical adjustment of this size gap. Molecules are introduced by some form of self assembly into the gap between the two electrodes. The presence of the molecules in the gap cannot be observed directly but is inferred from the conductance properties. Using statistics over many contact-breaking cycles and representing the data in 2D histograms in many cases gives a clear signature of the molecular junctions.

In order to investigate the mechanism of electron transport in more detail advanced probes are needed. Recently we have developed break junction devices with a third electrode in the form of an electrostatically coupled gate. In one realisation of these devices the gate can be used to operate a single-atom switch. In a second variant the transport across a single molecule can be tuned by the gate potential. Experiments were performed on a series of porphyrin-based compounds, which show sharp resonances in the differential conductance spectrum. We found that these resonances shift in position as a function of the gate potential, while they also shift as a function of the distance between the (source and drain) electrodes, which we refer to as “mechanical gating”. The combination of the two effects allows us to identify the origin of the effects.

Invited talk Thursday 16:20

Structured epitaxial graphene

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Abstract

The original concept of graphene electronics focused on carbon nanotube properties. Carbon nanotubes were known to be high mobility ballistic, phase coherent conductors and quantum confinement effects produced significant band gaps. However, it turns out to be very difficult to develop nanotube electronics platform for a variety of reasons including fundamental physical constraints related to the quantum mechanical properties of the metal-to-nanotube contacts. Graphene electronics can in principle overcome the major problems because graphene structures can be patterned using conventional lithography and dissipation at contacts can be controlled. However, these developments rely on the premise that narrow, ballistic graphene ribbons can be produced. Experiments on conventionally patterned graphene structures produced from graphene that is deposited on insulating substrates have been discouraging. The graphene ribbon mobilities are so low due to edge roughness effects, to render this direction to be impracticable. On the other hand, graphene produced on silicon carbide turns has been found to be more immune to edge scattering problems. This effect is explained in terms of a topologically protected edge state that are in fact expected in essentially all graphene ribbons with reasonably straight edges. Moreover, recent developments of template grown graphene structures on silicon carbide are promising. Very narrow ballistic graphene ribbons that demonstrate electronic phase coherent properties, have been produced with these methods which again brings the original concept of graphene based nanoelectronics back into play. Recent developments in the science and technological implications of epitaxial graphene nanostructures will be presented.

Quasi-particle interference mapping of electronic states in clean and Bi-covered fcc (111) surfaces

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Abstract

STM does not only allow to imagine the atomic structure, but spectroscopic modes give also access to the electronic properties of surfaces. Recently, the so-called quantum interference mapping technique has been employed to observe spatial oscillations of the energy-resolved density of states which originate from elastic scattering between two momentum eigenstates of the sample, $k_{\mathrm{i,f}}$ [1]. The resulting oscillation exhibits a wave vector which corresponds to the scattering vector $q(E) = k_{\mathrm{i}}(E) + k_{\mathrm{f}}(E)$. Analysis of those scattering events allows to get insight into the dispersion relations and spin polarization [2]. We have focused on $\sqrt{3} \times \sqrt{3}\,\mathrm{Bi/Ag}(111)R30°$, a spin-split Rashba system. On this surface we observed spectroscopic features, that are assigned to two Rashba-split bands. Quantum interference mapping shows that backscattering is not only allowed below but also above the Rashba energy. We argue that the observed behavior can be understood within the Bloch picture where k refers to the crystal momentum and the velocity of an electronic state is defined as $v_n(E) = \frac{1}{\hbar}\nabla_k E_n(k)$. The analysis of the energy dispersion of scattering channels reveals a conventional Rashba splitting for the unoccupied Rashba bands, while
hybridization is observed in the occupied states.

[1] M. F. Crommie, C. P. Lutz, and D. M. Eigler, Nature **363**, 524, (1993)
[2] Pedram Roushan, Jungpil Seo, Colin V. Parker, Y. S. Hor, D. Hsieh, Dong Qian, Anthony Richardella, M. Z. Hasan, R. J. Cava, and Ali Yazdani, Nature**460**, 1106, (2009)

Invited talk Friday 8:40

Effect of charge disorder on the conduction along the edge of a two-dimensional topological insulator

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Abstract

Static charge disorder may create electron puddles in the bulk of a material which nominally is in the insulating state. A single puddle - quantum dot - coupled to the helical edge of a two-dimensional topological insulator enhances the electron backscattering within the edge. The backscattering rate increases with the electron dwelling time in the dot. While remaining inelastic, the backscattering off a dot may be far more effective than the proposed earlier inelastic processes involving a local scatterer with no internal structure. We find the temperature dependence of the dot-induced correction to the universal conductance of the edge and use our theory to assess the effect of static charge disorder on the electron transport along the edge.

Surface Optical Spectroscopy of Metal Nanostructures

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Abstract

Optical spectroscopy is a powerful and nondestructive tool for in situ studies of condensed matter including tiny structures on surfaces. Optical conductivity tensor elements can be determined by polarization sensitive extinction measurements. The frequency dependence of these elements informs about the various electronic and vibrational excitations. For low-dimension systems, only little is known about the spectral behavior of the dynamic conductivity from collective electronic excitations. In the interband range, observed optical transitions in combination with theory can help to identify atomic structures. Further support for structural identification comes from vibrational spectroscopy, for example Raman scattering from metal-atom structures on semiconductor substrates. We will give some examples on ultra-high vacuum studies of optical spectra of systems in the focus of FOR 1700 [1,2,3] and others that demonstrate the sensitivity of the method, e.g. [4].

[1] S. Chandola et al., Phys. Rev. Lett. 102, 226805 (2009).
[2] E. Speiser et al., Phys. Stat. Sol. B 247, 2033 (2010).
[3] C. V. Hoang et al., Appl. Phys. Lett. 96, 243101 (2010).
[4] J. Pischel et al., J. Phys. Chem. C 116, 14014 (2012).

Ultrafast Dynamics of CDW systems probed by time-resolved ARPES

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Abstract

The electronic properties of complex materials are often governed by strong electron-phonon coupling and many-body correlation effects leading to phenomena like metal-insulator transitions or superconductivity and the formation of broken symmetry ground states. One example for the coupling between electronic and phonon degrees of freedom are phase transitions in charge-density wave (CDW) materials where at low temperature a periodic lattice distortion leads to an opening of an electronic gap at the Fermi surface. Ultrafast optical excitation can induce non-equilibrium phase transitions as well as electronic and geometrical structure changes of such complex materials on femtosecond timescales.

We use time- and angle-resolved photoemission spectroscopy (trARPES) for a systematic study of the tri-telluride CDW system (RTe3, R=Te, Ho, Dy) to probe directly the resulting transient evolution of the electronic structure and the collective phonon dynamics of the system through their influence on the quasiparticle band structure. Furthermore we investigate the prospects of low-energy excitations (coherent phonons or magnons) to optically control and probe transient states of matter: Examples are the control of the amplitude mode in DyTe3 by two-pulse excitation and THz pumping of optical magnons in NiO by the magnetic field of light.

Photoelectron spectroscopy of organic layers and interfaces: from orbital mapping to Kondo resonances

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Abstract

Structurally well-defined model systems are irreplaceable for the investigation of the peculiar physical properties of organic solids and interfaces. I will show how ultrathin organic films allow a very precise analysis of the electronic structure by means of angle resolved photoelectron spectroscopy (ARPES). On the example of organic dyes on metal surfaces I will demonstrate that the interaction at the interface leads to several new states which can crucially influence the charge transport properties [1]. The influence of the interfacial bonding leads to the generation of metal-molecule hybrid states, which can be identified by analyzing the angular intensity distribution in the photoelectron spectra [2]. This method allows a mapping of the electronic wave functions and thus provides unique information about molecular orbitals [3]. The mixing of molecular orbitals with delocalized substrate states leads to very interesting phenomena inthese hybrid systems. As a consequence the molecules communicate laterally via the substrate. This can be observed by a substantial banddispersion of the hybrid band and thus to a delocalization of molecular states mediated bythe substrate [4].Moreover, I will demonstrate that the hybridization of localized with delocalized statesleads to very sharp excitation features at the Fermi level. These signals display a strongtemperature dependence and are immediately connected to the binding energy of themolecular states, determined by the coupling between the molecule and the substrate[5,6]. At low temperatures, the line-width, appearing on top of the partly occupiedhybridization state, amounts to only ~ 10 meV, representing an unusually small energyscale for electronic excitations in these systems. I will show that this observation can beexplained by a generalized Kondo scenario.

[1] Y. Zou*et al.* Surface Science, 600(6): p. 1240-1251 (2006).
[2] J. Ziroff*et al.* Physical Review Letters 104 (2010)
[3] M. Dauth*et al.* Physical Review Letters, 107(19): p. 193002 (2011).
[4] M. Wiessner*et al.* Nature Communications (in press).
[5] A. Schöll*et al.* Science, 329(5989): p. 303-305 (2010).
[6] J. Ziroff*et al.* Physical Review B *Rapid communications*, 86, 045417 (2012).

Competing phases of the Hubbard model on a triangular lattice - insights from the entropy

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Abstract

Based on the ladder dual-fermion approach, we present a comprehensive study of the phases of the isotropic Hubbard model on the triangular lattice. We find a rich phase diagram containing most of the phases that have already been experimentally observed in systems where the interplay between geometric frustration and electronic correlations is important: paramagnetic metal, paramagnetic insulator, Mott-insulator with 120° antiferromagnetic and a non-magnetic insulating state, i.e. possibly a spin liquid state. This establishes that the Hubbard model on frustrated lattices can serve as a minimal model to address the intricate interplay of frustration and correlation. We also show that entropic considerations can be successfully used for understanding many striking features of the triangular systems, such as the large thermo power found in NaxCoO2 · yH2O.

Poster contributions

The poster session will be held in front of the lecture hall

1. STM-controlled contacting and lifting of single molecules
E. Tartaglini, J.M. van Ruitenbeek, F. Galli, *Kamerlingh Onnes Laboratories, Leiden*
R. Eelkema, C. Maity, *TU Delft Chemical Engineering*

2. Detection of vibration mode scattering in electronic shot noise
Manohar Kumar, R. Avriller, A. Levy Yeyati, and Jan M. van Ruitenbeek
University Leiden

3. Fano-Kondo effect in a parallel double quantum dot
Rodrigo Agundez, Miriam Blaauboer, and Sven Rogge
Technical University Delft

4. The Quantum Highway: Episode I - Accidents, traffic jams and standing Bloch Waves
René Heimbuch and Harold J.W. Zandvliet, *University of Twente*

5. Exact prefactors in correlation functions of one-dimensional quantum liquids
MiłoszPanfil, SebasEliëns, and Jean-Sébastien Caux
Institute for Theoretical Physics, Universiteit van Amsterdam

6. Rare earth silicide nanowires on silicon surfaces
Mario Dähne and Stephan Appelfeller, *TU Berlin*

7. Optical and Vibrational Properties of Au Nanowires on Ge(001)
Norbert Esser, Eugen Speiser, Jochen Räthel, Arne Baumann, Sandhia Chandola
ISAS Berlin

8. Surface Phonons and Phase Transition of In-Nanowires on Si(111) surfaces
Norbert Esser, Eugen Speiser, Jochen Räthel, Arne Baumann, Sandhia Chandola, *ISAS Berlin*

9. Ag/Si(557): Tailoring of 1D plasmon dispersion by doping
Christian Brand, Ulrich Krieg, *Leibniz Universität Hannover*

10. Electronic properties of graphene nanoribbons
Frederik Edler and Jens Baringhaus, *Leibniz Universität Hannover*

11. Self-assembled model system to explore 1D physics on Si(001):H
Christoph Renner and Francois Bianco, *University of Geneva*

12. Epitaxial grown Kondo lattices spanning different localization regimes of the Ce 4f electrons
Holger Schwab, *Universität Würzburg*

13. Quantifying the one-dimensionality in Lithium purple bronze: 6-band NMTO tight-binding compared to ARPES
LenartDudy, *Universität Würzburg*

14. Numerical simulations of a model for topological Kondo insulators
Jan Werner, *Universität Würzburg*

15. Dimensional-crossover-driven Mott transition in the frustrated Hubbard model
MarcinRaczowski, *Universität Würzburg*

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