Physics at the borderline between 1D and 2D

Bad Honnef

1-3 March 2017

NWO

DFG Deutsche Forschungsgemeinschaft

Introductory remarks

The present workshop on "Physics at the borderline between 1D and 2D" follows the long-standing tradition of the annual Aschermittwochs-Rundgespräche. It is the second workshop with the same title as four years ago, intended not only to demonstrate the progress made in the field, but also, by exploiting the homely atmosphere of the (freshly renovated and extended) Physikzentrum, to bring together young and experienced scientists for exchange of ideas and thorough discussions.

The workshop is based on the collaboration of three research initiatives. These three are closely related. The Sonderforschungsbereich 1170 “Topological and Correlated Electronics at Surfaces and Interfaces” (ToCoTronics) aims at combining two of the most active and exciting fields of modern condensed matter physics: topological phases of matter and strong electronic correlations. In recent years, the two fields themselves have developed to an advanced level with a deep understanding of the underlying physics. The combination of the two fields, i.e. the presence of both spin orbit interaction (the basis of topological phases of matter) and strong electronic correlations, is a typical problem of low-dimensional systems.

The main objective of the FOM program, which comes to an end with this final meeting, was 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. While these topics have close and obvious connections to the research program of SFB1170, they also have many similarities with the central task of the research unit FOR1700, funded by DFG, which 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. In other words, the peculiar properties of ideal one-dimensional (1D) electronic systems, such as quantization of conductance, charge-density waves (CDWs), and Luttinger liquid behavior, with a variety of instabilities and a wealth of associated phase transitions serve as basis and theoretical reference. The main - and still largely unsolved – question is how these properties are modified by 2D and 3D interactions in the “real” world. Controlled manipulation of these interactions by structure, chemical reaction and impurities may give access to the underlying physics.

The program of this workshop combines overview talks in this field by renowned experts on various aspects with reports on recent progress by the participating groups. We hope very much that they serve as incentive for lively discussions, which may continue not only during coffee breaks, but even up to late at night in the Bürgerkeller.

Program Overview

Wednesday, March 1, 2013

After 13:00		Arrival at Physikzentrum Bad Honnef
14:00		Meeting PIs FOR 1700
15:00	Welcome	
15:15- 16:00	Thierry Giamarchi (invited)	1D phenomena, the theorist's view
16:00-16:30	Eric Jeckelmann	Peierls insulators and Luttinger liquids in atomic wires on substrates.
16:30-17:00		Coffee break
17:00-17:30	Norbert Esser	Opt. Methods in quasi-1D systems
17:30 -18:00	Connor Hogan	Ab initio simulations of structural and optical properties of Au-stabilized Si(hhl) surfaces
18:00 – 18:30	Herbert Pfnür	Plasmon excitations and transport in atomic wires
18:30 – 19:00	Stephan Appelfeller	From 2D to 1D - Tb silicide nanowires on Si(hhk)
19:00	Buffet-style dinner	

Thursday,	**March 2, 2017**	
7:45	Breakfast	
8:30-9:00	Michael Horn v. Hoegen	1D Atomic Wires at Surfaces: Phase Transitions and Ultrafast non-Equi-librium Structural Dynamics in the Si(111)-In (8x2)<>(4x1) System
9:00- 9:30	Andreas Lücke	Grand canonical Peierls transition in In/Si(111): Soft phonons, electronic states and chemical bonds
9:30-10:00	Martin Wolf	Transient Electronic Band Structure Mapping by Time-resolved ARPES: The In/Si(111) (8x2) ↔ (4x1) Phase Transition
10:00-10:30	Coffee break /Posters	
10:30-11:15	Jörg Kröger (invited)	Exploring electron transport through low-dimensional structures with a scanning tunnelling microscope
11:15-11:45	Paolo Sessi	Visualizing the universal response of Dirac materials to perturbations
11.45 -12.15	Jean-Sébastian Caux	Searching for Luttinger liquid physics: from theoretical promises to experimental challenges
12:15-14:00	Lunch	
14.00 -14.45	Sven Rogge (invited)	Engineered quantum matter
14:45 - 15.30	Paul Snijders (invited)	Modulation doping of a low-dimensional correlated electron system
15:30 – 16:00	Coffee break /Posters	
16:00 - 16:30	Mariusz Krawiec (invited)	Purely one-dimensional spin-orbit split bands in Pb/Si(553) surface

16:30 - 17:00	Manuel Ligges	Structural dichroism and anisotropic scattering dynamics in non-linear photoemission from Pb nanowire arrays on Si(557)
17:00-19:00	Poster session	
From 19:15	Buffet-style conference dinner	

Friday March 3, 2017

7:45	Breakfast	
8:45 - 9:30	Toru Hirahara (invited)	Inducing magnetism in topological insulators by self-organized incorporation of a ferromagnetic layer
9:30 - 10.00	Jörg Schäfer	Synthesis and Spectroscopy of Bismuthene - From 2D to 1D Physics
10:00 - 10:30	Paul Koenraad	Magnetic interactions in artificially created Mn assemblies in a GaAs (110) surface
10:30 - 11.00	Coffee break	
11:00 -11:30	Johannes Jobst	Probing the interaction between atomically thin layers in Van der Waals systems
11:30 - 12:00	Domenico DiSante	Robust spin-polarized midgap states at step edges of topological crystalline insulators
12:00 - 12:30	Hendrik Bentmann	Probing the wave-function anatomy of spin-orbit coupled surface states: spin polarization, orbital texture, and hybridization
12:30	Lunch	End of Workshop

Miscellaneous

Breakfast **7:45**

Lunch **12:50 – 14:30**

Buffet-style Dinner **from 19:00**

Internet

To access the wireless LAN service provided by the Physikzentrum connect to the visible access point with SSID PBH and use the following password:
011235813 “the first 8 Fibonacci numbers (not digits)”
encryption WPA-2 personal

For participants without laptops there is a computer room on the ground floor with 4 windows computers (2 English & 2 Deutsch), password pbh.

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

From 1D to 2D: dimensional crossover

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One-dimensional quantum systems exhibit physical properties quite different from their higher dimensional counterparts. In particular they are described by the paradigmatic Tomonaga-Luttinger liquid (TLL) fixed point. The TLL exhibit a set of properties ranging from powerlaw correlations, fractionalization of excitations, and topological and non-local excitations. I will discuss some of the experimental realizations in which TLL can be obtained both in the condensed matter realm and in cold atomic systems.

The set of TLL properties is extremely sensitive to the coupling between 1D systems and if it is clear that such systems should ultimately recover the physics of higher dimensional systems how this dimensional crossover takes place is still largely a mystery. I will review the techniques to tackle such a problem, and some of the experimental situations in which we can probe such dimensional crossover.

Peierls insulators and Luttinger liquids in atomic wires on substrates

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Abstract
Quasi-1D electron systems can be realized in good approximation in linear atomic wires deposited on the surface of a semiconducting substrate. The interpretation of experiments with theories for 1D systems is often controversial, however. A fundamental issue is that we have a poor understanding of the effects of the coupling between an atomic wire and its 3D substrate on phenomena such as the Peierls instability or the Luttinger liquid behavior of 1D conductors. We discuss two investigations of this issue.

First, the grand-canonical Peierls transition is analyzed thoroughly within the Su-Schrieffer-Heeger (SSH) model. Starting from a generalized SSH-like model inferred from first-principles simulations, we show that the metal-insulator transition in In/Si(111) can be seen as a first-order grand canonical Peierls transition in which the substrate acts as an electron reservoir for the wires. This approach explains naturally the existence of a metastable metallic phase over a wide temperature range below the critical temperature and the sensitivity of the transition to doping.

Second, we propose 3D lattice models for isolated atomic wires on substrates and show that they can be mapped onto narrow ladder models that can be investigated with well-established methods for 1D correlated systems. This approach is illustrated with a systematic study of a wire with a Hubbard-type coupling using the density-matrix renormalization group and quantum Monte Carlo simulations. We show that typical 1D features can be observed in these models, such as Mott insulators with gapless spinon excitations and 1D conductors with Luttinger liquid behavior. Thus effective narrow ladder models provide us with a promising approach to investigate correlation effects in wire-substrate systems.

References:

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Atomic Scale Interface Analysis by Raman Spectroscopy: Clean and Adsorbate Terminated Semiconductor

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Abstract
Raman spectroscopy is widely applied in material sciences, (bio-) chemistry, life sciences etc. to study the vibrational properties and correspondingly the structure of molecules, nanostructures, and various inorganic and organic materials. Due to recent improvements in instrumentation Raman scattering nowadays allows to study material properties on the nanoscale. Thus Raman spectroscopy is nowadays even suitable for the analysis of surface atomic structures by analysing surface phonons, i.e. vibrational modes confined to the few uppermost layers of a surface.

Within FOR1700 we have been systematically using Raman spectroscopy in order to deliver structure sensitive spectroscopic fingerprints as a very specific information for structural details of the metal nanowires. In correlation with according ab-initio calculations atomic structures have been analysed. Examples comply not only the In/Si(111) system, but also Au/Si(111), Pb/Si(111) and most recently Au on stepped Si surfaces (Si(553)). In all of these systems surface confined modes have been identified in the Raman spectra. For In/Si(111) a full understanding of the vibrational properties has been achieved over recent years. Still relevant is the temperature related phase transition and adsorbate induced modifications. The vibrational properties of Pb on Si(111) are still in discussion, also Au on Si(553). In particular the ab-initio modelling of these structures is very demanding.
Future work within FOR1700 will concentrate on adsorbate induced modifications of metal (Au, In) nanowires on Si(hhk).

Ab initio simulations of structural and optical properties of Au-stabilized Si(hhl)

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Abstract

The adsorption of gold on flat and stepped Si(111) surfaces induces regular and spatially-dense nanostructure arrays, through formation of single or multiple atomic Au chains within the terraces as well as rows of Si dangling bonds and honeycomb structures at the step edge [1]. These reconstructions constitute a well-defined prototype for studying a range of interesting phenomena in (quasi-)one dimensional systems including metal-insulator transitions, long-range spin order, Rashba splitting, and spin chain manipulation [2,3]. Ab initio simulations have been used to predict surface structure, investigate such phenomena and interpret experimental results [4,5]. One such technique that offers precise microscopic insight is reflectance anisotropy spectroscopy (RAS), which is particularly sensitive to the intrinsically anisotropic nature of surface structural motifs (Au chains, spin chains, adatoms, and so on) [6,7]. In this presentation I will demonstrate how careful simulations of RAS experiments carried out within the FOR1700 network yields insight into structural and electronic phenomena in these systems and even how to control them externally [8].

References:

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Plasmon excitations and transport in atomic wires

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Abstract

Plasmons in low-dimensional systems respresent an important tool for coupling energy into nanostructures and the localization of energy on the scale of only a few nanometers. Contrary to ordinary surface plasmons of metallic bulk materials, their dispersion goes to zero in the long wavelength limit, thus covering a broad range of energies from terahertz to near infrared, and from mesoscopic wavelengths down to just a few nanometers.

The typical starting point are two-dimensional (2D) metallic layers. As demonstrated, tuning of their dispersion is possible by changes of charge carrier concentration or effective masses in the partially filled 2D conduction bands. These dispersion curves are shown to be linearized by coupling to other electron gases (2D or 3D), but also by introduction of anisotropy, e.g. by regular arrays of steps (leading also to partial localization of the plasmons). In systems, such as arrays of gold chains on regularly stepped Si surfaces, only the dispersion is 1D, whereas shape and slope of the dispersion curves depend on the 2D distribution of charge within each terrace and on coupling between wires on different terraces. In other words, the form of the confining quasi-1D potential enters directly into the 1D plasmon dispersion and gives new opportunities for tuning.

Low-dimensional plasmons are directly related to electronic surface transport. Therefore, we will concentrate on a comparison of plasmonic and transport properties in quasi-1D systems such as Au/Si(hhk) and Pb/Si(557).

From 2D to 1D – Tb silicide nanowires on Si(hhk)

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Abstract

The deposition and annealing of Tb on Si surfaces leads to a variety of fascinating nanostructures from zero-dimensional clusters on Si(111) [1] over one-dimensional nanowires on Si(001) [2,3] to well ordered two- and three-dimensional Tb silicide layers on Si(111) [1,4]. The metallic Tb disilide monolayer on Si(111) is especially interesting since its formation pins the Fermi level near the Si conduction band minimum making it interesting for ohmic contacts on *n*-type Si or as infrared detectors on *p*-type Si. Its electronic structure near the Fermi level is characterized by sharp bands forming a hole pocket at $\bar{\Gamma}$ and strongly anisotropic electron pockets at the $\bar{M}$ points [2]. For monolayer depositions on Si(hhk) surfaces being vicinal to Si(111), the formation of nanowires with widths depending on the offcut angle is expected.

In this work, the growth and the electronic structure of such Tb disilicide nanowires on vicinal Si(111) surfaces were studied with scanning tunneling microscopy (STM) and angle resolved photoemission spectroscopy (ARPES). In general, narrower Tb disilicide structures are observed for larger offcut angles, but the morphology of these structures strongly depends on the offcut direction. For Si(hhk) surfaces with h < k, the silicide forms well defined nanowires with sharp edges (see figure 1), while only irregular stripes are formed for h > k.

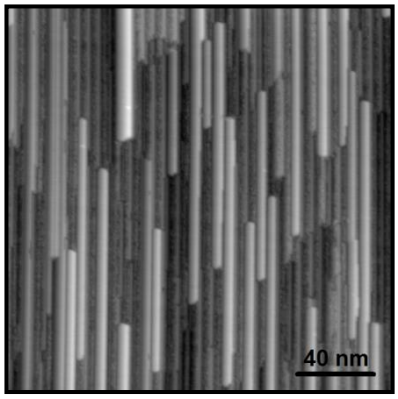

Figure 1 STM image of Tb silicide nanowires on Si(557).

Nevertheless, the characteristic two-dimensional electronic structure of the disilicide monolayer is observed with ARPES on all vicinal surfaces. Thereby, the bands, which were sharp for the extended monolayer on planar Si(111), broaden in the direction perpendicular to the step edges due to the confinement of the silicide structures to finite widths. This effect is quantified by an analysis of the electron pockets at the $\bar{M}$ points.

Furthermore, electronically purely one-dimensional bands emerge for low Tb coverage on Si(335). Tb silicide structures possibly corresponding to these bands are discussed.

This work was funded by the DFG, FOR1700, project E2.

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

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Abstract
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 and opening of a bandgap. 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 330 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. 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. 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 [4,5] 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.

These results were obtained in close collaboration with A. Lücke, S. Sanna, U. Gerstmann, S. Wippermann*), and W.G. Schmidt from Paderborn University and A. Samad Syed, V. Miksic Trontl, I. Avigo, P. Zhou, M. Ligges, and U. Bovensiepen from Duisburg-Essen University.

References:

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Grand canonical Peierls transition in In/Si(111): Soft phonons, electronic states and chemical bonds

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Abstract

Density functional theory calculations on the intensively studied In/Si(111)(4x1)/(8x2) nanowire array are used to illustrate how strongly structural, vibrational and electronic properties of atomic-scale wires are intertwined. Soft phonon modes transform the nanowire structurally between the insulating hexagon structure and metallic In zigzag chains. Optical excitation changes the potential energy surface of the In nanowires and may melt the charge-density wave far below the critical temperature [1,2]. The femtosecond dynamics of the charge-density wave melting is rationalized by ab initio molecular dynamics on ground- and excited-state potential energy surfaces. In addition, a detailed bonding analysis gives a comprehensible visualization of the underlying physics.

The results presented in this talk were obtained in close collaboration and partially in direct response to experimental work performed by the Horn-von Hoegen and Bovensiepen group in Duisburg.

References:

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Transient Electronic Band Structure Mapping by Time-resolved ARPES: The In/Si(111) (8x2) ↔ (4x1) Phase Transition

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Abstract

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 (RTe_3) compounds we can directly map the dynamics of opening and closing of the CDW gap and identify at least two Peierls-like amplitude modes [1]. Furthermore, we have developed high-harmonic-driven XUV photoemission at 500 kHz repetition rate to allow complete access to the Brillouin zone in trARPES studies [2].

Here 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 boundary is observed to close already after 200 fs, while states at the zone center shift from above to below the Fermi level within 500 fs. Moreover, the structural transition into the (4x1) phase, as manifested by the splitting of the m_2-m_3 bands, is completed after 700 fs. We conclude that the insulator-to-metal transition and the structural transition occur on distinct time scales suggesting a more complex scenario than a “standard” Peierls mechanism.

A recent combined DFT and Raman study of the thermally induced transition [3] points strongly to a Peierls-like scenario, whereby (1) a combination of shear and rotary distortions leads to the opening of band gaps and spectral shifts at specific points in the band structure and (2) variations of the substrate induced chemical potential (with temperature, doping or photoexcitation) plays a crucial role. However, in our trARPES study we observe a coherent phonon mode around 2.4 THz (80 cm^{-1}), but no coherent modulation by the amplitude mode(s) as in the RTe_3 compounds [1]. The absence of a coherent excited amplitude mode suggests a non-standard mechanism for the phase transition, which is discussed in the context of recent time-resolved electron diffraction results [4].

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Exploring electron transport across low-dimensional structures with a scanning tunnelling microscope

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Abstract

A scanning tunnelling microscope is used to form contacts to single atoms and molecules adsorbed on surfaces. Electron transport across such junctions is then studied for a variety of material combinations.

Junctions composed of non-magnetic tips, Co and Ir atoms on a ferromagnetic Fe ultrathin film exhibit ballistic anisotropic magnetoresistance. The magnetization-dependent mixing of atomic d-orbitals with different symmetries due to spin-orbit coupling can account for the observations [1].

Upon closing tunnelling junctions across a normal-metal tip and the surface of a conventional superconductor the gradual evolution of the Bardeen-Cooper-Schrieffer energy gap to a zero-bias peak is observed. The zero-bias enhancement of the junction conductance is ascribed to Andreev reflection that depends on the atomic-scale details of the junction geometry [2].

Wrinkles and blisters of graphene on a metal surface exhibit extraordinarily high signals of graphene phonons in inelastic electron tunnelling spectroscopy. The reduced graphene-metal hybridization in partly delaminated wrinkles and blisters together with the phonon-mediated mixing of nearly-free and Dirac electron bands is suggested as an explanation [3].

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Visualizing the universal response of Dirac materials to perturbations

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Abstract
The discovery of topological insulators represents a milestone in condensed matter physics. It twisted the way we look at the band structure of solids classifying them in terms of well-defined global invariants of their bulk wavefunction electronic space. When non-trivial, these invariants are associated to the emergence of Dirac boundary modes which, because of their topological origin, are protected against weak disorder.
In my talk, I will provide an overview of universal trends characterizing topological materials interacting with external perturbations.
I will start by discussing topological insulators interacting with time-reversal symmetry breaking perturbations. I will demonstrate that, contrary to the general belief, magnetic order and gapless states can coexist. I will show that this unexpected behavior is associated to a dual nature of the dopants, which gives rise to a two-fluid behavior with opposite and competing trends.
I will then report more recent results on Weyl semimetals, showing how their interaction with atomic scale perturbations give rise to strong and universal spectroscopic signatures associates to their topological states, i.e. Weyl points and Fermi arcs.

Searching for Luttinger liquid physics: from theoretical promises to experimental challenges

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Abstract

Current realizations of quasi-one-dimensional electronic gases in semiconductor nanowires and self-assembled atomic wires provide a renewed playground for investigating the peculiar physics of Luttinger liquids, associated to well-known expectations such as spin-charge separation of electronic excitations at low energies. This talk will provide an overarching theoretical review of the fundamentals of Luttinger liquids, including their application in various other low-dimensional contexts such as quantum magnets, cold atomic gases and atomic wires. Besides presenting a number of recent theory developments including extension to higher energies, threshold singularities in response functions and exact correlation prefactors, we will discuss the numerous outstanding challenges associated to actually observing this type of physics in the laboratory.

Engineered quantum matter

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Abstract.
Atomic-scale engineering reached the level of control where single-atom devices can be reproducibly fabricated with high yield [1]. This talk focuses on the progress of single dopant atom placement in the context of engineered quantum matter. Silicon offers a particularly interesting platform for single dopants because when isotopically purified it acts as a "semiconductor vacuum" for spins. This leads to extraordinary coherence [2] that is used to realise donor atom based qubits [3]. Spatially resolved tunnelling experiments reveal the spectrum and quantum state image of such qubits [4]. These measurements grant access to the wavefunction of donors in the silicon lattice that exhibited quantum interference processes reflecting the valley degrees of freedom inherited from the silicon "semiconductor vacuum". This interference process makes it possible to pinpoint the dopants to their exact position in the lattice [5] which is essential in the evaluation of engineered quantum matter. Finally, a first step towards engineered quantum matter in for form of atomic chains was taken where interacting dopants were employed to simulate a two-site Hubbard Hamiltonian at low effective temperatures with single-site resolution. Quasi-particle tunnelling maps of spin-resolved states with atomic resolution reveal interference processes from which the entanglement entropy and Hubbard interactions are quantified [6].

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Modulation doping of a low-dimensional correlated electron system

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Abstract

Low-dimensional “complex” transition metal oxides have been at the heart of some of the most exciting discoveries in condensed matter research. Apart from temperature, the primary tuning parameter that is being exploited to access the often rich phase diagrams is charge doping through the introduction of dopant species, resulting in even more complexity in the materials. While most of these findings have been made in stoichiometrically complex oxides, we recently discovered that stoichiometrically “simple” materials such as RuO2 can host similar physics. In low-dimensional simple systems, however, dopants inevitably introduce structural defects, and property tuning of the “simple” parent system is thus very limited. In this talk, I will present our recent results in subsurface modulation hole doping of a “simple” 2D Mott-Hubbard insulating surface phase. By changing the chemical potential in the substrate, we observe a significant spectral weight transfer into a quasiparticle peak at the Fermi level, consistent with a hole doping level of up to 20%. Using scanning tunneling spectroscopy, we show that this hole-doped Mott insulator exhibits a strongly nested Fermi contour, and a van Hove singularity in the density of states just below the Fermi level, while a strong zero bias anomaly suggests that a superconducting or spin density wave anomaly emerges. If time permits, I will also discuss the emergence of a novel doping-induced phase transition in a 2D semiconducting bilayer. These results propel simple surface systems into view as model systems for “complex” physics generally found in bulk transition metal oxides.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Purely one-dimensional spin-orbit split bands in Pb/Si(553) surface

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Abstract

Vicinal (stepped) Si surfaces serve as templates to grow one-dimensional nanostructures [1]. Many of these systems have been extensively studied in relation to expected various exotic phenomena like Peierls metal-insulator transition, spin-orbit density wave, spin chains or one-dimensional diffusion of atoms [2-5].

Here we discuss structural and electronic properties of quasi-one-dimensional Pb structures prepared on Si(553) surface [6,7]. The scanning tunneling microscopy study show regular distribution of terraces separated by monatomic steps. Each terrace consists of a five-atom-wide nanoribbon. The spin- and angle-resolved photoemission spectroscopy ((S)ARPES) measurements and density functional theory (DFT) calculations reveal peculiar electronic structure with multiple surface bands crossing the Fermi level along the direction parallel to step edges and a small gap in the perpendicular direction. As shown by SARPES and DFT these bands are spin-polarized, composed of p_x orbitals, and decoupled from the rest of the system. The experimentally observed spin splitting of the bands yields 0.6 eV at room temperature, which is the largest found to now in the Si-based metallic nanostructures, and makes the Pb/Si(553) system a promising candidate for applications in spintronic devices.

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

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Structural dichroism and anisotropic scattering dynamics in non-linear photoemission from Pb nanowire arrays on Si(557)

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Abstract

We investigate the dynamics of unoccupied electronic states in Pb/Si(557) nanowire arrays as a function of in-plane electron momentum $\boldsymbol{k}_{||}=(k_x,k_y)$ using femtosecond time- and angle-resolved two-photon photoemission. Two unoccupied electronic states at E-E_F=3.30 eV and E-E_F=3.55 eV are observed that exhibit momentum-averaged life times exceeding those in 2D quantum well states in monolayer Pb/Si(111) by four and three times, respectively [1]. Along the direction perpendicular to the wires (k_y), life time contributions from inelastic intra- and interband scattering as well as from elastic scattering (dephasing) can be disentangled by a momentum-resolved analysis of the ultrafast dynamics [2]. The direction parallel to the wires (k_x) yields more complex dynamics that are accompanied by linear dichroic effects that point towards an uneven angular in-plane symmetry of the corresponding electronic bands. This finding might help to partially confirm or rule out structural models for this system that are currently under discussion.

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Inducing magnetism in topological insulators by self- organized incorporation of a ferromagnetic layer

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Abstract

Inducing magnetism into topological insulators is intriguing not only in terms of exploring exotic phenomena such as the realization of the quantum anomalous Hall effect (QAHE) [1,2], but also for technological applications. While most studies have focused on doping magnetic impurities to open a gap at the surface-state Dirac point, many undesirable effects have been reported to appear that makes it difficult to determine whether the gap opening is due to the time-reversal symmetry breaking or not [3,4]. Here we have succeeded in generating a massive Dirac cone in a heterostructure which was fabricated by co-deposition of Mn and Se on top of the Bi_2Se_3 surface. Our experimental results, supported by relativistic *ab initio* calculations, demonstrate that the self-organized heterostructure shows ferromagnetism up to room temperature and a clear Dirac-cone gap opening of ~100 meV without any other significant changes in the rest of the band structure. It can be considered as a result of the direct interaction of the surface Dirac cone and the magnetic layer rather than a magnetic proximity effect. This spontaneously formed self-assembled heterostructure with a massive Dirac spectrum, characterized by a nontrivial Chern number C=-1 [4], has a potential to realize the QAHE at high temperatures than reported up to now.

This work has been done in collaboration with Sergey V. Eremeev (Tomsk, Russia), Tetsuroh Shirasawa (AIST, Japan), Yuma Okuyama (Tokyo Tech., Japan), Takayuki Kubo, Ryosuke Nakanishi, Ryota Akiyama, Akari Takayama, Shuji Hasegawa (University of Tokyo, Japan), Tetsuya Hajiri, Shin-ichiro Ideta, Masaharu Matsunami, Yasumasa Takagi, Kiyohisa Tanaka, Toshihiko Yokoyama, Shin-ichi Kimura (UVSOR, Japan), Kazuki Sumida, Koji Miyamoto, Taichi Okuda (HiSOR, Japan), and Evgueni V. Chulkov (DIPC, Spain).

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Synthesis and Spectroscopy of Bismuthene - From 2D to 1D Physics

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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. In our current study combining experiment and theory we demonstrate that the room-temperature regime, manifest in a large bulk energy gap, can be achieved by a new quantum spin Hall paradigm. In contrast to the previous mechanisms at work in graphene and HgTe, respectively, our approach specifically exploits the on-site atomic spin-orbit coupling as a third avenue. It is based on a substrate-supported monolayer of the high-Z element bismuth, and is experimentally realized as a honeycomb lattice of "bismuthene" on top of the insulator SiC(0001). Consistent with theory, we detect a huge bulk gap of ~0.8 eV and conductive edge states [1]. Our results demonstrate a concept for a quantum spin Hall wide-gap scenario, where the chemical potential resides in the global system gap, ensuring robust edge conductance.

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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. 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 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].

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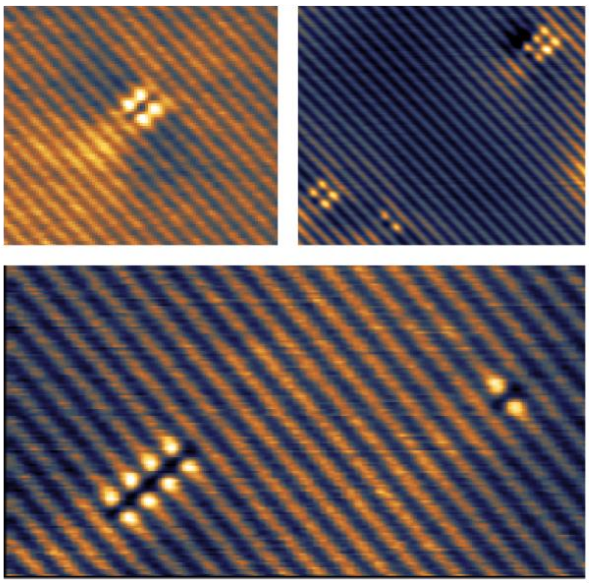

Fig. 1: Examples of assemblies of Mn atoms in the 110 surface of GaAs that have been created by STM manipulation.

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Probing the interaction between atomically thin layers in Van der Waals systems

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Abstract

Many layered materials can be mechanically exfoliated, down to atomically thin sheets. This opens the possibility to stack different layers together to form systems with novel properties: the so-called van der Waals (vdW) materials. Clearly, the extent to which these properties differ from those of the mother materials is governed by the interaction between the different layers. If there is considerable overlap, a new band structure may be formed, encoding all key properties of the vdW material. However, in other cases, the interaction is preferably negligible, e.g. allowing one to isolate graphene from a substrate below. All in all, understanding the quantum overlap between different sheets is key to help us to create materials with custom-designed properties in the future. Here, we investigate interlayer interactions using a novel technique, focusing on graphene and hexagonal boron nitride (hBN).

Experimentally, the occupied bands, that is, the filled electron states below the Fermi level, can be routinely measured. However, it has been remarkably difficult to characterize the empty part of the band structure. We have developed a method to do just that, based on low-energy electron microscopy (LEEM) [1]. The technique, named angle-resolved reflected-electron spectroscopy (ARRES), relies on the dependence of the reflectivity of low-energy electrons on both their kinetic energy and their incident angle on the sample. It has a high cross-section and a spatial resolution of ~10 nm, which is five orders of magnitude better than other techniques.

Applying ARRES to flakes of few-layer graphene and hBN separately, we find quantization of the conduction band into well-defined interlayer states for both systems. These interlayer states have a similar dispersion and very similar energies for the two materials. Nevertheless, in a stack of graphene on hBN, we observe no coupling of the electronic systems of the two materials despite their intimate contact. This substantiates that hBN is an excellent substrate to isolate graphene from its environment over a wide energy range.

The possibility to perform both ARRES and ARPES (angle-resolved photo-emission spectroscopy) in our LEEM facility ‘ESCHER’, will give us the opportunity to investigate band structure formation in a large range of VdW systems in the near future. Knowledge on this is crucial to tailor the properties of Van der Waals crystals, stacked in a LEGO-like fashion.

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Robust spin-polarized midgap states at step edges of topological crystalline insulators

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Abstract

Topological crystalline insulators are materials in which the crystalline symmetry leads to topologically protected surface states with a chiral spin texture, rendering them potential candidates for spintronics applications. In this talk, I report on the discovery of one-dimensional midgap states at odd-atomic surface step edges of the three-dimensional topological crystalline insulator (Pb,Sn)Se. A minimal toy model and realistic tight-binding calculations identify them as spin-polarized flat bands connecting two Dirac points. The midgap states inherit stability through the two-dimensional Dirac metal from the three-dimensional bulk insulator. This makes (Pb,Sn)Se the first example for a crystal symmetry-protected hierarchy of one- and two dimensional topological modes, which we experimentally prove to result in a striking robustness to defects, strong magnetic fields, and elevated temperature.

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Probing the wave-function anatomy of spin-orbit coupled surface states: spin polarization, orbital texture, and hybridization

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Abstract

Spin-polarization of electronic states at the surfaces and interfaces of materials with strong spin-orbit interaction currently attracts wide interest in condensed matter physics, *e.g.* in the context of topological insulators. Angle-resolved photoelectron spectroscopy (ARPES) directly probes the band dispersion of these states and –via the transition matrix element of the photoemission process– even allows one to address the spin-dependent properties of their wave functions. Here, I will present recent ARPES studies of topological insulators and related spin-orbit coupled materials where systematic variation of polarization and frequency of the exciting light are combined with high energy resolution and spin-resolved photoelectron detection. I will discuss specific examples where this experimental approach could provide detailed insight into the "anatomy" of the spin-orbit coupled wave functions, namely their spin-polarization and orbital textures in momentum space [1] as well as hybridization effects [2].

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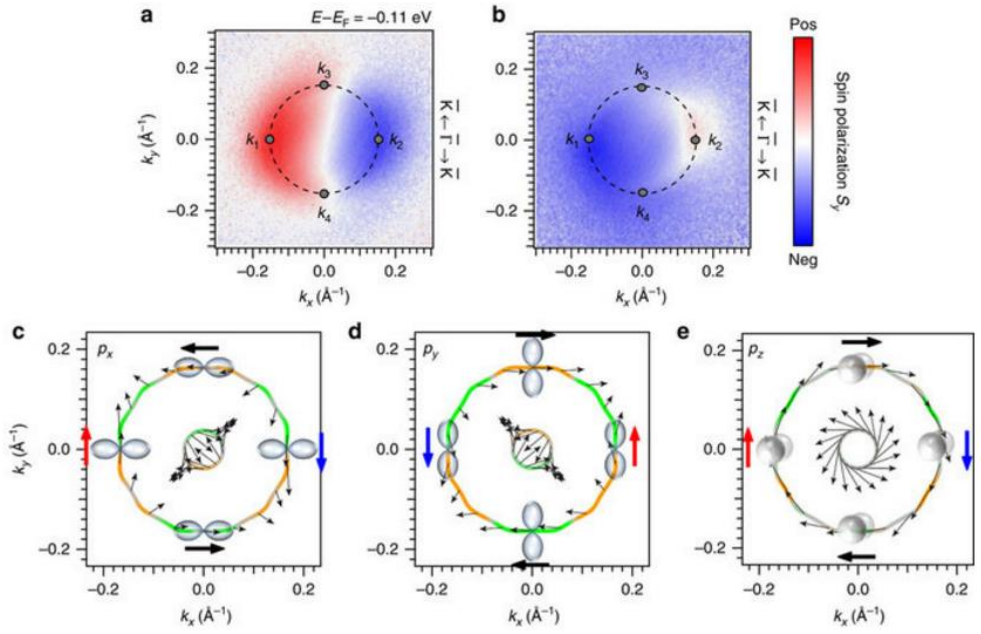

Figure 1: Spin-resolved ARPES data of spin-orbit split electronic states in the polar semiconductor BiTeI(0001) for (a) s-polarized and (b) p-polarized light. (c)-(e) First-principles calculation of the spin-polarization and the orbital character of the electronic states [1].

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

Poster contributions

1. **Vibration eigenmodes of the Au-(5 × 2)/Si(111) surface studied by Raman spectroscopy and first-principles calculations**
2. **Si(hhk)-Au: Structural, electronical and vibrational properties calculated from first principles**
3. **Surface transport in a quantum spin liquid system**
4. **Functionalization of Si(553)-Au surface with hydrogen and small organic molecules**
5. **Tuning the conductivity along atomic chains by selective chemisorption**
6. **Functionalization of Si(553)-Au with hydrogen and small organic molecules**
7. **Two-dimensional crossover in one-dimensional plasmons in Si(hhk)-Au**
8. **Tb induced 1D and 2D nanostructures on Si(111)**
9. **The power of collaboration: Tb silicide nanowires on Si(001) investigated**
10. **Density functional theory investigation Of rare earth silicide nanowires**
11. **Strain-induced quasi-one-dimensional rare-earth silicide structures on Si(111)**
12. **Quantitative LEED studies on Si(111)-(5x2)-Au**
13. **Silicon nanoribbons on Ag(110): silicene or Si chain reconstruction?**
14. **Band-Edge Exciton Fine Structure and Recombination Dynamics in InP/ZnS Colloidal Nanocrystals**
15. **Edge states at vacancy islands on pristine Ni(111)**
16. **Spin-orbit coupling and hybridization effects at metal and topological insulator surfaces**
17. **Quantum size effect in ultra-thin Bismuth films: The crossover between 3D- and 2D behavior**
18. **Charge-ordered state in the low-temperature phase of Pb/Si(111)**
19. **Polarization-dependent non-linear photoemission study of unoccupied electronic states in Pb-Si(557) system**
20. **Quasi-1D Materials Probed by Photoemission: Dimensional Crossover in NbSe3 and Ultrafast Peierls Transition in In/Si(111) Nanowires**

21. **Pinning of topological solitons at extrinsic defects in a quasi one-dimensional charge density wave**
22. **Atomic structure of self-organizing iridium induced nanowires on Ge(001)**
23. **A two-dimensional Dirac material on a band gap substrate: Germanene on MoS2**
24. **Germanene: the germanium analogue of graphene**
25. **Electric field induced delamination of 2D layered materials**
26. **Gold-induced Surfaces on Stepped Germanium: Growth and Characterization**
27. **New topological surface state in occupied electronic structure of α-Sn**
28. **Hydrogen etching of SiC(0001): Route to an epitaxy template**
29. **Synthesis and Spectroscopy of Bismuthene**
30. **Ultrafast Electron Diffraction: Lattice Response of Ultrathin Pb Layers and Islands on Si(111) upon Optical Excitation**
31. **Spin correlations in the Si(553)-Au nanowire system**
32. **Ultrafast non-thermal switching of a surface CDW system in the regime of critical damping**
33. **Epitaxial Sn on h-BN terminated ZrB_2**

Poster Abstracts

1. Vibration eigenmodes of the Au-(5 × 2)/Si(111) surface studied by Raman spectroscopy and first-principles calculations

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Ordered submonolayers of adsorbate atoms on semiconductor surfaces are a popular playground for electronic correlation effects, which are tightly connected to the local atomic arrangement and the corresponding vibrational eigenmodes. Among the investigated systems, the Au-covered Si(111) surface has been characterized extensively, yet different structural models are under debate [1,2,3,4]. In this poster, we report on a study of the vibrational properties of the Si(111) surface with Au-induced (5 × 2) reconstruction using polarized Raman spectroscopy and first-principles calculations [4]. Upon Au coverage, the vibrational eigenmodes of the clean reconstructed Si(111)-(7 × 7) surface are quenched and replaced by new phonon modes, determined by the Au-(5 × 2) reconstruction. Several polarization-dependent surface eigenmodes emerge in the spectral range from 25 to 120cm^{-1}, with the strongest ones at 29, 51, and 106 cm^{-1}. In our first-principles calculations we have determined the vibrational frequencies, the corresponding elongation patterns, and the Raman intensities for two different structure models currently discussed in the literature. The best agreement with the experimental results is achieved for a model with 0.7 monolayer coverage and seven Au atoms per unit cell, proposed by S. G. Kwon and M. H. Kang [4].[1] S. Erwin, Phys. Rev. Lett. **91**, 206101 (2006).
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2. Si(hhk)-Au: Structural, electronical and vibrational properties calculated from first principles

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Self-assembled atomic-scale Au wires on vicinal Si(hhk) surfaces have become popular model systems for the realization of quasi one-dimensional physics. Despite numerous experimental and theoretical studies there are still open questions concerning their structural and electronic properties.
Here we present a systematic exploration of the Si(775)-Au surface in dependence on the Au coverage based on density-functional theory. For the most stable structures the electronic properties are calculated. Interestingly, we find the energetically most favored models to show a magnetic ordering, similar to the case of Si(553)-Au or Si(557)-Au.
The oxygen adsorption energetics and the influence of oxygen on the electronic properties of Si(553)-Au and Si(557)-Au are calculated. It is found the Si ad- and rest-atoms on Si(557)-Au provide energetically favored adsorption sites, which substantially alter the transport along the wire direction. Since this structural motif is missing on Si(553)-Au, the transport channels remain almost unaffected by oxidation in this case. This explains recent transport measurements by the Tegenkamp and Pfnür group.

Finally, the vibrational properties of Si(553)-Au and Si(111)-Au are calculated within the frozen phonon approximation. Several surface localized modes are found that are well suited to explain recent Raman data by the Esser and Geurts groups.

3. Surface transport in a quantum spin liquid system

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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(553) 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].
By means of low energy electron diffraction (LEED) and 4-tip STM, 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 transport experiments done at various temperatures were performed with a squared probe geometry, thus being sensitive to the crystallographic directions [2]. After subtracting the isotopic contribution of carbon-impurity induced p-type doped space-charge-layer, we clearly revealed 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]. Apparently, the magnetic ordering, originating from localized dangling bond states of the Si honeycomb lattice, is not feeding back to the 1D electronic states at Fermi energy.
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4. 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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5. Tuning the conductivity along atomic chains by selective chemisorption

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Atomic chain ensembles grown by self-assembly are prototype 1D systems, which are expected to exhibit outstanding electronic properties, e.g. Peierls instabilities or Luttinger liquid behavior [1]. Recently, the Au-induced atomic chain structures on Si(hhk) attracted a lot of attention. The strong spin-orbit coupling gives rise to spin polarized surface bands and in case of Si(553)-Au even quantum spin liquid behavior [2,3]. However, such properties can strongly be altered by imperfections, e.g. defects induced by adsorbates.
In this contribution, we present a systematic study of the transport properties of Si(553)-Au and Si(557)-Au system by means of a 4-tip STM system in combination with SPA-LEED. In particular, we studied the influence of molecular oxygen on the surface conductivity. Our DFT calculations suggest that the origin of metallic surface bands along the wires are strongly dependent on the structural building blocks. Moreover, the modeling shows that the ad- and rest-atoms on Si(557)-Au provide energetically favored adsorption sites, which predominantly alter the transport along the wire direction. Since this structural motif is missing on Si(553)-Au, the transport channels remain almost unaffected by oxidation.

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

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Atomic metallic chains on vicinal Si substrates can be used as templates for the growth of hybrid molecule-solid nanostructures. The advantage of these structures 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. Hydrogen is able to drive a reversible metal-insulator transition on the Si(553)-Au surface and also changes the adsorption geometry of organic molecules[1], extending the functionalization possibilities of the surface.
We use surface-sensitive and polarization-sensitive optical techniques, such as Raman Spectroscopy (RS), Reflection Anisotropy Spectroscopy (RAS) and Infrared Spectroscopic Ellipsometry (IRSE) to establish a direct connection between optical spectra and surface structure via ab-initio calculations[2]. Optical fingerprints allow us to gain information on structural and electronic properties of the system.
The plan for the future is the realization of highly ordered molecular array geometries and the understanding of charge transfer between molecules and atomic wires. This will open possibilities for further functionalization through modification of terminal groups of molecules. Furthermore, the possibility to explore different chemical conditions between elementary organic molecules and surfaces at the nanoscale offer a new point of view for studies of complex biological molecules.

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7. Two-dimensional crossover in one-dimensional plasmons in Si(hhk)-Au

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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 description and predictions of the behavior are still rather unsatisfactory. Several key aspects of the influence such as e.g. many-body effects as well as Coulomb screening are still rather unexplored. Additionally, (quasi-)one-dimensional (1D) electronic systems show unusual transport properties such as Peierl's transitions or Tomonaga-Luttinger liquid (TLL) behavior, that have a strong influence on the plasmonic properties.
For quasi-one-dimensional structures Au induced wires on regularly stepped Si(hhk) offer the perfect playground with their varying terrace widths. Additionally, adsorption of metals like e.g. Ag [1], or Au can induce various forms of wire structures. In this study, we prepared the systems to a state, where each of these terraces hosts a gold chain [2,3].
For our investigations, spot profile analysis in low energy electron diffraction (SPA-LEED) allowed checking the wire quality. 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.
Despite the metallic 1D character, the plasmon dispersion strongly depends on a two-dimensional crossover: on the lateral distribution of the 1D electron density of states (DOS) within one terrace (intrawire correlation), as well as on the spacing of the wires (interwire correlation). The description of these results is possible by a modified plasmon model for an array of quasi-1D metallic channels. We obtained effective widths which are considerably smaller than the terrace widths. Also, tunneling spectroscopy measurements show a modulated DOS of similar diameter. These effective widths seem to be influenced both by the structural motif, i.e. single or double chain, as well as by the terrace size.
Within in this group of investigated wires, doping the systems with adatoms seems to be possible. Upon adsorption of atomic hydrogen, the plasmon dispersion redshifts in energy. Furthermore, for the systems hosting a Si-adatom chain, i.e. Si(557)-Au and Si(775)-Au, in an atmosphere of molecular oxygen, a blueshift takes place. These shifts can give further insight into the properties of adsorption sites on the surface that still need to be clarified.
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8. Tb induced 1D and 2D nanostructures on Si(111)

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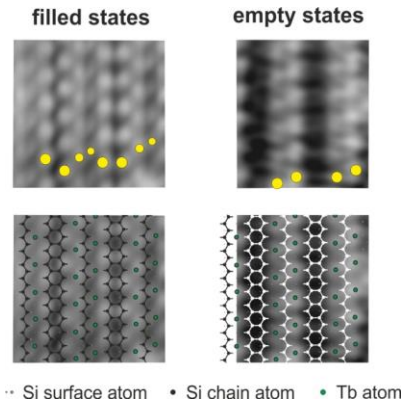

Similar to other trivalent rare earth metals, Tb forms very interesting silicide nanostructures on Si surfaces. A variety of mostly two-dimensional nanostructures, including clusters, submonolayer structures and layered films is observed on the Si(111) surface [1-3], while the formation of silicide nanowires is found on the Si(001) surface [4]. In this work, the growth of Tb silicide nanostructures on Si(111) from submonolayer to multilayer coverages is investigated using scanning tunneling microscopy (STM), angle resolved photoemission spectroscopy (ARPES), and density functional theory (DFT). Here, we concentrate on the 5×2 submonolayer structure and the 1×1 monolayer structure consisting of hexagonal $TbSi_2$.
For the quasi-one-dimensional 5×2 superstructure, a structure model consisting of alternating Si chains and rows of Tb atoms in between could be developed. This model, which is supported by DFT calculations showing a semiconducting behavior with strong electronic anisotropy, nicely explains the observed STM features as well as the different configurations (see Fig. 1). In contrast, the 1×1 superstructure formed in the case of one monolayer $TbSi_2$ clearly shows a two-dimensional metallic electronic structure with characteristic electron pockets at the $\bar{M}$ points and a hole pocket at the $\bar{\Gamma}$ point, similar to corresponding silicides formed from other trivalent rare earth metals.This work was funded by the DFG, FOR1700, projects E2 and T1.

Figure: Filled and empty states STM images of the Tb induced 5×2 superstructure together with the corresponding structure model.

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9. The power of collaboration: Tb silicide nanowires on Si(001) investigated

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One-dimensional metallic nanowires are fascinating due their unique physical phenomena, e.g. Tomonaga-Luttinger liquid behavior, and their possible implementation in future nanotechnology, e.g. as ultra narrow interconnects. Rare earth silicide nanowires on Si(001) represent a model system for one-dimensional metals that show a Peierls-like transition at low temperatures [1]. Here, we present an overview on the results on Tb silicide nanowires on Si(001), also obtained by intensive collaborations mostly within FOR1700 [2-6].
The growth of the nanowires and their structure were analyzed using scanning tunneling microscopy (STM) and low energy electron diffraction [2]. The nanowire growth is preceded by the formation of a 2x7 reconstructed wetting layer, which may stay intact upon nanowire formation. The structure of the nanowires could be identified as hexagonal Tb disilicide in agreement with our core-level photoemission data [3].
Reflectance anisotropy spectroscopy (RAS) is capable to differentiate between wetting layer and nanowire growth [4]. Thereby, the RAS spectra agree very well with the STM observations showing peaks associated with strain due to the nanowire formation especially for samples containing large bundles of nanowires and a negligible wetting layer.
The electronic properties of the nanowires were analyzed using scanning tunneling spectroscopy (STS) [3], transport measurements at nanowire bundles [5], and angle resolved photoemission spectroscopy (ARPES) [3]. STS and the transport measurements clearly reveal the metallic character of the nanowires and the Fermi surfaces obtained by ARPES show slightly oscillating lines indicating a quasi one-dimensional structure with weak interaction between neighboring nanowires.
Furthermore, high resolution transmission electron microscopy and scanning transmission electron microscopy with energy dispersive X-ray analysis demonstrated the possibility to passivate the nanowires by capping with Si, being a prerequisite for future applications [6].
This work was funded by the DFG, FOR1700, projects E2, E3, and E4.
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10. 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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11. Strain-induced quasi-one-dimensional rare-earth silicide structures on Si(111)

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Rare earth (RE) covered silicon surfaces have been in the focus of research for more than 30 years due to their unique properties. For instance, thin RE-silicide films on n-type Si(111) possess very low Schottky-barriers in conjunction with an abrupt surface making them interesting as ohmic contacts. Furthermore RE-silicide nanowires might be applicable as interconnects in future nanodevices or as plasmonic waveguides due to their quasi one-dimensional structure. Here, we report on the (2Ö3 x Ö3) R30° reconstruction for RE coverages exceeding 1 ML, which is therefore related to the well-known (Ö3 x Ö3) R30° reconstruction. We characterize the structure of the silicide films by means of Low Energy Electron Diffraction (LEED) including Spot Profile Analysis (SPA-LEED), Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) developing a complex model for the reconstructed surface including formation of quasi one-dimensional structures, due to striped domains.

12. Quantitative LEED studies on Si(111)-(5x2)-Au

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The (5x2)-Au reconstruction on Si(111) has been in the focus of research for nearly 50 years now. Lately, in particular as a prototype for one-dimensional (1D) metallic chain structures. In order to understand the physical properties accompanying these 1D chains a profound knowledge of the atomic structure is needed. Historically, a plethora of atomic structures (EBH [1],AN [2],KK [3]) with varying Au coverages were discussed. More recently Shirasawa et al. [4] were able to show that Surface X-ray Diffraction experiments favor the KK-model slightly. Due to the higher surface sensitivity of Low Energy Electron Diffraction (LEED) as compared to SXRD we carried out quantitative LEED experiments in order to assess this observation.

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13. Silicon nanoribbons on Ag(110): silicene or Si chain reconstruction?

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Since the first reported synthesis, in 2005, of one-dimensional nanoribbon structures following the evaporation of silicon on Ag(110), a number of studies have proposed that they are composed of silicene—a single layer of a buckled honeycomb structure of Si atoms [1]. This interpretation was subsequently questioned in experimental studies using Raman and surface differential reflectance spectrsocopy [2]. Recently a number of new structural models have been proposed that suggest a Si-stabilized missing row reconstruction based on zigzag [3] or pentamer [4] chains. Here I present refined experimental and theoretical studies using grazing incidence x-ray diffraction (GIXD), scanning tunneling microscopy (STM), surface optical spectra (RAS and SDRS), and density-functional theory (DFT) which confirms the correct structure as being a pentamer chain reconstruction and definitively ruling out a honeycomb structure like that of freestanding silicene [5].

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14. Band-Edge Exciton Fine Structure and Recombination Dynamics in InP/ZnS Colloidal Nanocrystals

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The interest in Cd-based technological applications is limited because of the high toxicity of Cadmium. Therefore, significant efforts are made to develop colloidal synthesis schemes yielding heavy-metal-free quantum dots. Among the potential materials, InP appears to be an ideal candidate since it has a band gap close to CdSe as well as a reduced toxicity. As fluorescence properties of semiconductor colloidal quantum dots are linked to the band-edge properties, it is essential to have a deep knowledge of their excitonic fine structure.
This work reports on a temperature-, time-, and spectrally resolved study of the photoluminescence of type-I InP/ZnS colloidal nanocrystals with varying core size. By studying the exciton recombination dynamics we assess the exciton fine structure in these systems. In addition to the typical quantum size effect, we observe a large (up to tens of meV) splitting between optically active ('bright') and optically passive ('dark') excitons due to strong electron-hole exchange interaction. This bright-dark splitting has a significant impact on the optical properties of band-edge excitons and leads to a pronounced temperature dependence of radiative decay. We also evidence a strong dependence of the spin-flip rate between bright and dark exciton states on the core size which represents a phonon bottleneck. Furthermore, our data show that the radiative recombination of the dark excitons scales linearly with bright-dark energy splitting for CdSe and InP nanocrystals. These findings strongly suggest a universal dangling bonds-assisted recombination of the dark exciton in colloidal nanostructures. For the future, it is planned to investigate the relaxation dynamics of photo-induced hot carriers in quasi-1D metal wires on semiconductors and strongly correlated systems.
This work has been supported by the Deutsche Forschungsgemeinschaft via Sonderforschungsbereich TRR 160 and the Russian Science Foundation.
Publication:
L. Biadala et al., *ACS Nano*, 2016, 10 (3), pp 3356-3364, DOI: 10.1021/acsnano.5b07065

15. Edge states at vacancy islands on pristine Ni(111)

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Recently, the dispersion relation of surface electronic states of pristine Ni(111) has been probed by quasiparticle interference (QPI) [1]. In agreement with earlier inverse photoemission experiments [2] an exchange-split and upward dispersing Shockley-type *sp*-derived surface state was observed. In a follow-up investigation we have studied the electronic properties of step edges surrounding hexagonally shaped vacancy islands by means of low-temperature scanning tunneling spectroscopy. Our results indicate that *A*- or *B*-steps are markedly different. While one type of step edge is essentially featureless, local tunneling spectra measured on the other exhibit an additional peak. By comparison with density functional theory calculations we discuss if this peak can potentially be interpreted as a one-dimensional edge state.
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16. Spin-orbit coupling and hybridization effects at metal and topological insulator surfaces

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Spin-orbit coupling at surfaces gives rise to spin-polarized electronic bands, induced, *e.g.*, by the Rashba effect at metal surfaces or by a non-trivial topology in topological insulators. Here, we shall provide an overview about recent angle-resolved photoemission experiments on different metal and topological insulator surfaces. First, we will discuss the role of hybridization between spin-polarized surface states and the underlying bulk continuum, which can acquire a spin-dependence and affect spin-orbit splitting sizes, as well as dispersion and scattering rates of the electronic states [1,2]. Second, based on several case studies, we will discuss how and to what extent spin-resolved photoemission experiments can grant insight into the spin and orbital character of spin-orbit split states [3,4].

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17. Quantum size effect in ultra-thin Bismuth films: The crossover between 3D- and 2D behavior

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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 temperature and magnetic field dependent transport. The conductance G at low temperature is mainly governed by surface states while at higher temperatures activated transport from bulk channels sets in. We have carefully analyzed the G(T)-behavior of films as a function of thickness. With decreasing film thickness d, the bulk gap was found to increase with d^{-1}, as expected due to the quantum size effect. High quality films with large grain sizes, so that the electron mean free path is much larger than the film thickness, are mandatory to observe the confinement effects in an electronic transport experiment.

Moreover, angle dependent magneto-conductance measurements for various thicknesses were performed. In particular, 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 that are involved [2]. For all thicknesses $G_{par.}(B)$ is dominated by weak-anti-localization (WAL). As the film thickness decreases the coupling strength between the interfaces increases. 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 bulk carriers involved in the transport. However, a transition from WL to WAL for the thinnest film (20 BL) has been observed, so that any interaction between surface and bulk states can be neglected in this thickness regime indicating truly two dimensional transport.

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18. Charge-ordered state in the low-temperature phase of Pb/Si(111)

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Two-dimensional triangular lattices of Group IV adatoms on diamond lattice substrates provide a rich playground for experimental studies and many-body calculation techniques. For the system investigated in this work, 1/3 monolayer of Pb on Si(111), preceeding studies have noted a phase transition from $\sqrt{3}\times\sqrt{3}$ to 3×3 at 86 K [1]. In our high-resolution scanning tunneling microscopy and spectroscopy measurements in the low-temperature phase, we have unveiled the formation of a charge-ordered state by carefully mapping the local density of states. Furthermore, we find a structural rearrangement with a 2-up/1-down configuration. These results are supported by state-of-the art many body calculations using the Variational Cluster Approach (VCA), which is sensitive to both spin- and charge-densitiy wave instabilities. I will present a comparison of our measurements and the latest results from VCA calculations.

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19. Polarization-dependent non-linear photoemission study of unoccupied electronic states in Pb-Si(557) system

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Strong correlations exist between the electronic properties and geometries of low dimensional systems. Metallic nanowires grown on vicinal Si surfaces are example of such systems whose structural anisotropy and transition from higher to lower dimensions at a critical temperature make them interesting for investigation. Pb nanowires grown on stepped Si (557) surface is one of such systems which undergo a transition from being 2-dimensionally semiconducting to one-dimensional metallic phase [1]. We aim at understanding the electronic structure and dynamics of electrons taking place in this system by using femtosecond time- and angle-resolved two photon photoemission.

Earlier 2PPE revealed two unoccupied electronic states at E-E_F = 3.55 and 3.30 eV, respectively. Density functional theory calculations reveal that these states are spatially located predominantly on the lead wires and are decoupled from the Si substrate. We further find momentum-averaged lifetimes of 24 and 35 fs of these two states, respectively. The photoemission yield and the population dynamics depend on the electron momentum component perpendicular to the steps of the Si substrate. The momentum-dependent dynamics cannot be described by means of rate equations leading to the conclusion that momentum- and direction-dependent dephasing of the electronic excitations, likely caused by elastic scattering at the step edges on the vicinal surface, modifies the excited-state population dynamics in this system [2]. We also used 2PPE to characterize the symmetry of the higher lying state by polarization-dependent measurements. The 2PPE intensity of this state exhibits an interesting intensity dependence on light polarization. For pump-polarization change, it is found to (i) be different along positive and negative momentum directions $+k_x$, $-k_x$ along the steps, respectively, and (ii) show a dependence along $-k_x$ that is inverted after rotating the surface by π around the surface normal, while it remains along $+k_x$. Similar effects of different 2PPE intensity are observed for probe polarization change along $+k_x$, $-k_x$ and also inverted dependence for π rotated sample, along $-k_x$. However, along $+k_x$, unlike pump-polarization change case, no clear intensity dependence is found which might be an indication of broken final state symmetry. Given a local $\sqrt{3}\square\sqrt{3}$ surface structure [1] we conclude that our observation is consistent with a superposition of a six-fold and a three-fold symmetry of the electronic Pb-Si hybrid state, potentially due to two coexisting atomic structures at the interface.

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20. Quasi-1D Materials Probed by Photoemission: Dimensional Crossover in NbSe3 and Ultrafast Peierls Transition in In/Si(111) Nanowires

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In one spatial dimension (1D), reduced screening and a restricted phase space for scattering heavily impact the electronic properties of materials due to the ensuing strong correlations. In real materials, coupling to higher dimensions results in quasi-1D behaviour, characterised by a crossover energy or temperature above which excitations exhibit 1D character, while low-energy excitations behave as in a Fermi liquid and ordered phases such as charge density waves commonly occur [1]. Here we report the investigation of two quasi-1D systems using high-resolution ARPES and state-of-the-art time-resolved ARPES respectively.
NbSe3 is an archetypical linear-chain compound, which undergoes incommensurate charge density wave (CDW) transitions at T_1 = 145 K and T_2 = 59 K [2]. Our high-resolution angle-resolved photoemission spectroscopy (ARPES) study finds evidence of a dimensional crossover from 1D to 3D as a function of decreasing energy and/or temperature. From the warping of the Fermi surface a crossover energy scale of around E_C = 120 meV is extracted based on a tight-binding model. This is corroborated by an analysis of the density of states which reveals 1D behaviour only above E_C. The data presented here attest an intermediate regime in which the bosonisation expected for a purely 1D dispersion is still partially observed while approaching the Fermi-liquid regime of 3D coherence. Such an approach is in principle completely general, and we therefore expect the analysis presented here to be applicable to other quasi-1D materials.
Quasi-1D In/Si(111) nanowires undergo a structural transition from a (4x1) to an (8x2) unit cell at around 120 K, concomitant with a metal-to-insulator transition. Here we investigate the ultrafast photoinduced insulator-to-metal transition in In/Si(111) nano-wires by time-resolved ARPES. 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 boundary is observed to close already after 200 fs, while states at the zone centre shift from above to below the Fermi level within 500 fs. Moreover, the structural transition into the (4x1) phase, as manifested by the splitting of the m_2-m_3 bands, is completed after 700 fs. We conclude that the insulator-to-metal transition and the structural transition occur on distinct time scale suggesting a more complex scenario than a “standard” Peierls mechanism.
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21. 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 at- tention. 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. Financial support from the German Research Foundation (DFG), grant No. FOR1700 is gratefully acknowledged.

22. Atomic structure of self-organizing iridium induced nanowires on Ge(001)

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The atomic structure of self-organizing iridium (Ir) induced nanowires on Ge(001) is studied by density functional theory (DFT) calculations and variable-temperature scanning tunneling microscopy. The Ir induced nanowires are aligned in a direction perpendicular to the Ge(001) substrate dimer rows, have a width of two atoms and are completely kink-less. Density functional theory calculations show that the Ir atoms prefer to dive into the Ge(001) substrate and push up the neighboring Ge substrate atoms. The nanowires are composed of Ge atoms and not Ir atoms as previously assumed. The regions in the vicinity of the nanowires are very dynamic, even at temperatures as low as 77 K. Time-resolved scanning tunneling microscopy measurements reveal that this dynamics is caused by buckled Ge substrate dimers that flip back and forth between their two buckled configurations.

23. A two-dimensional Dirac material on a band gap substrate: Germanene on MoS_2

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To date germanene has only been synthesized on metallic substrates. A metallic substrate is usually detrimental for the two-dimensional Dirac nature of germanene because the important electronic states near the Fermi level of germanene can hybridize with the electronic states of the metallic substrate. Here we report the successful synthesis of germanene on molybdenum disulfide (MoS_2), a band gap material. Pre-existing defects in the MoS_2 surface act as preferential nucleation sites for the germanene islands. The lattice constant of the germanene layer (3.8 ± 0.2 Å) is about 20% larger than the lattice constant of the MoS_2 substrate (3.16 Å). Scanning tunneling spectroscopy measurements and density functional theory calculations reveal that there are, besides the linearly dispersing bands at the *K* points, two parabolic bands that cross the Fermi level at the Γ -point.

24. Germanene: the germanium analogue of graphene

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Recently, several research groups have reported the growth of germanene, a new member of the graphene family. Germanene is in many aspects very similar to graphene, but in contrast to the planar graphene lattice, the germanene honeycomb lattice is buckled and composed of two vertically displaced sub-lattices. Density functional theory 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, the relativistic variant of the Schrödinger equation. Germanene is a very appealing two-dimensional material. The spin-orbit gap in germanene (~24 meV) is much larger than in graphene (<0.05 meV), which makes germanene the ideal candidate to exhibit the quantum spin Hall effect at experimentally accessible temperatures. Additionally, the germanene lattice offers the possibility to open a band gap via for instance an externally applied electrical field, adsorption of foreign atoms or coupling with a substrate. This opening of the band gap opens the door to the realization of germanene based field-effect devices. In this topical review we will (1) address the various methods to synthesize germanene (2) provide a brief overview of the key results that have been obtained by density functional theory calculations and (3) discuss the potential of germanene for future applications as well for fundamentally oriented studies.

25. Electric field induced delamination of 2D layered materials

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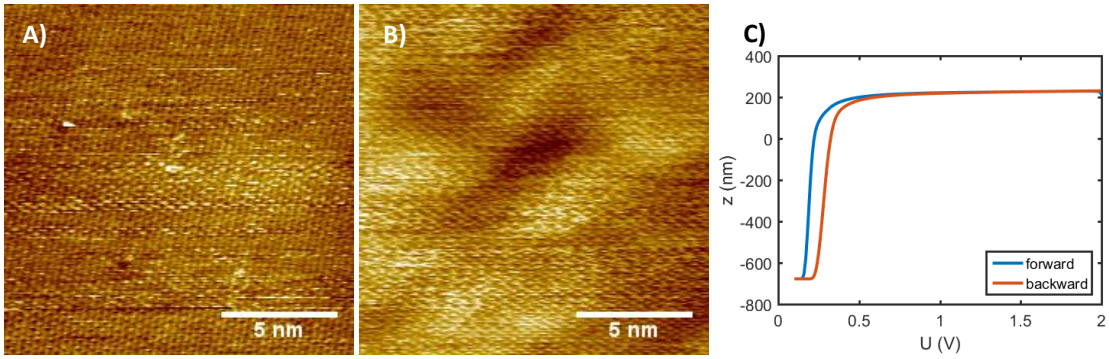
Two-dimensional (2D) systems have gained significant attention since it was discovered that atomically thin layers could be produced by mechanical exfoliation as first demonstrated on graphene, the two-dimensional allotrope of graphite.[1] Graphite and other 2D systems, such as the layered transition metal dichalcogenides (TMD), consists of 2D covalently bonded layers that are held together by weak van der Waals forces.[2] We demonstrate that, depending on the applied tip-sample bias voltage (and thus the electrostatic force), the surface of one of the TMD's, namely molybdenum disulfide (MoS_2), appears to have different topography. At a positive applied voltage, the top MoS_2 layer is completely stretched and the surface appears to be flat. In contrast, in the negative bias, the surface is puckered. This puckered surface is reminiscent of the surface of free-standing graphene.[3] This behavior and the relation between the applied bias voltage and the stretching of the MoS_2 has shown to cause the layers to be pulled up to hundreds of nanometers.This poster will provide experimental evidence for the delamination of 2D layered materials in the presence of a biased STM tip. A theory is proposed to describe the relevant attractive electrostatic forces between tip and sample and the opposing restoring forces of the membrane. Also the tunneling conditions to enhance or suppress the lifting behavior are discussed.



Figures: a) At a tip-sample bias voltage of 2V the top layer of MoS_2 appears to be flat, b) while for a bias of -2V the layer becomes puckered. c) Ramping the voltage over a range of 2V to 0.1V, with the feedback loop enabled, reveals that the top layer is lifted by hundreds of nanometers.

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26. Gold-induced Surfaces on Stepped Germanium: Growth and Characterization

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Adsorption of gold atoms on stepped Ge(hhk) surfaces leads to the formation of atomic wires via self-organization. Inspired by interesting physics such as spin chains on the step edges of similar gold-induced Si(hhk) surfaces [1], we establish recipes for the preparation of several gold-induced Ge(hhk) surfaces. Therefore, the preliminary sputter and anneal treatment of the stepped Ge(335), Ge(557) and Ge(553) substrates as well as the adsorption procedure of gold atoms provided by an electron beam evaporator have been optimized to achieve well- ordered surfaces. Due to the adsorption of gold atoms some Ge(hhk) surfaces undergo a refacetting in order to form a stable gold-induced surface. Based on scanning tunneling microscopy and low-energy electron diffraction we determine the formation of surface reconstructions on the atomic scale on the Ge(hhk)-Au surfaces. In particular, we have characterized these surfaces regarding the formation of atomic wire structures, such as those formed by the Au and Ge atoms, and will present first indications for the occurence of superstructures.

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27. New topological surface state in occupied electronic structure of α-Sn

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Electronic structure of α-Sn thin films strained compressively in the in-plane direction was studied by means of combined experimental and theoretical methods. Soft-X-Ray angular resolved photoemission spectroscopy (SX-ARPES), *ab-initio* GW calculations and *ab-initio*-based tight-binding (TB) calculations were used to investigate the occupied electronic band structure of the surface and sub-surface layers of this monoelemental topological material. SX-ARPES measurements being more bulk-sensitive reveal the ordering of bulk bands at the Γ-point, as well as the presence of an additional deeper-lying topological surface state (TSS). The latter appears between the projected bulk Γ_7^- and Γ_7^+ states and possesses *surface-resonance* character due to hybridization with bulk bands, in contrary to a surface-localized TSS near EF [1]. The topological character of this additional TSS is confirmed by unravelling the necessary band inversion and calculating the topological invariants for the occupied bulk electronic states. In agreement with the experimental data, semi-infinite TB calculations reproduce the bulk-derived character of the second TSS, with a maximum of the LDOS in the $\sim 3^{rd}$ unit cell below the surface.

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28. Hydrogen etching of SiC(0001): Route to an epitaxy template

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The hexagonal (0001) surface of silicon carbide offers a huge play-ground for the epitaxy of a variety of different materials. An intriguing aspect is the growth of honeycomb lattices made of high-Z elements, such as Sn or Bi, predicted to exhibit topological protected edge states. To enable successful epitaxy of such materials, one has to focus on the substrate quality, and prepare defect-free and well-ordered flat surfaces. In-situ gas phase etching in a hydrogen atmosphere makes it possible to achieve these required qualities.
Here we demonstrate the effects of different etching parameters studied by scanning tunneling microscopy. The results are analyzed regarding large-scale terrace formation and defect density. In general, the etched substrate surface becomes hydrogen-passivated which, however, impedes the bonding of the admitted high-Z atoms. One approach to hydrogen desorption from SiC(0001) discussed in the literature is a photoinduced process with synchrotron UV light.
In addition, we present the successful thermal desorption of hydrogen and the formation of a dangling bond (DB) state, as inspected by photoemission. The surface density of the DB state is analyzed in an annealing study. This finally renders SiC as a versatile growth template

29. Synthesis and Spectroscopy of Bismuthene

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The hunt for quantum spin Hall materials with large band gap is one of most vivid fields of contemporary solid state physics. In all systems reported so far, the bottleneck, preventing the use of the dissipationless currents with spin-momentum locking inherent in those materials for device applications, was their small energy gap, requiring very low operation temperatures. Despite other approaches, graphene with its honeycomb lattice geometry always fascinated the research community. In order to enlarge the bandgap, several theoretical proposals for heavy atom honeycomb lattices, e.g. with tin, have been made and attracted great attention. However, these proposals were made for non-existing, free-standing material.
We report the realization of a honeycomb lattice of a high-Z element, namely bismuth, which is synthesized on the wide-bandgap substrate SiC(0001) [1]. Scanning tunneling microscopy
imaging of “bismuthene” clearly displays the honeycomb structure, both in the occupied and
unoccupied states of the sample. Using tunneling spectroscopy, we find a huge bulk gap of ~800 meV, with the Fermi level positioned well inside this gap. Interestingly, metallic edge states are observed when the edge of the Bi film is approached. Both findings are consistent
with theoretical expectations. A comparison of angle-resolved photoemission measurements
and density functional theory band structure calculations is further manifesting the formation
of bismuthene. To understand the empirical electronic properties we performed a detailed theoretical analysis. A low-energy effective model demonstrates that the substrate not only stabilizes the Bi film, but plays a crucial role in the formation of the observed band gap, which is driven by the large on-site spin-orbit coupling.
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30. Ultrafast Electron Diffraction: Lattice Response of Ultrathin Pb Layers and Islands on Si(111) upon Optical Excitation

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Applying time resolved Reflection High Energy Electron Diffraction (tr-RHEED) we studied the excitation of the phonon system of thin Pb films and nanoscale islands on Si(111) upon impulsive IR irradiation. In a pump-probe scheme the sample is pumped by a fs-laserpulse at a wavelength of 800 nm. The lattice response of the sample is probed by a photo-generated electron pulse at an electron energy of 30 keV. Surface sensitivity is achieved by gracing incidence of the high energy electrons ($\vartheta < 6°$).

Pb islands and films were prepared *in-situ* on a Si(111) surface by molecular beam epitaxy. Deposition at low substrate temperatures $T < 100$ K results in a layer-by-layer growth mode of epitaxial films with a thickness which can be as low as 4 monolayers. In contrast, at higher substrate temperatures the growth mode changes to the preferred Stranski-Krastanov mode where on top of a wetting layer islands start to grow. The height of these nanoscale islands is electronically stabilized and thus either 3, 5, or 7 Pb monolayers.

Upon fs-laserpulse irradiation the electron system of the Pb films or islands is excited. Subsequently electron-phonon coupling causes an enhanced incoherent motion of the Pb atoms, i.e., an increase of lattice temperature which is observed through a transient drop of diffraction intensity due to the Debye-Waller effect. As Pb is known to have a strong electron-phonon coupling $g_\infty = 12.4 \times 10^{16}$ Wm^{-3}K^{-1} in the bulk, the time constant of the energy transfer to the lattice system is expected to be of the order of 800 fs in the framework of a simple two-temperature-model. In contrast, experimentally a rather slow time constant of $\tau_{surf} = 3.2$ ps was observed at the surface of thin Pb films resulting in a strongly reduced coupling constant of $g_{surf,TTM} \approx 2.9 \cdot 10^{16}$ Wm^{-3}K^{-1}. Additionally, no thickness dependency of the heating time constant τ_{surf} was found albeit the ultrathin Pb layers exhibit quantum well states, which strongly affect the electronic system.

In the case of small Pb islands the gracing incidence geometry causes diffraction in transmission geometry of the high energy electrons. This provides access to bulk information of the vertically and laterally confined islands. Surprisingly, a lattice response with a time constant of $\tau_{islands} = 4.6$ ps was observed for all island heights, which is even slower than at the surface of the films ($g_{islands,TTM} \approx 2 \cdot 10^{16}$ Wm^{-3}K^{-1}). These results demonstrate how reduced dimensionality of spatially confined systems affects the lattice response under intense optical excitation and thus the coupling of the electronic and phononic subsystems.

31. Spin correlations in the Si(553)-Au nanowire system

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Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand chains per Si terrace with a twofold periodicity along the wire. These metallic wires are structurally terminated by Si step edge atoms, which exhibit a three-fold periodicity of half-filled dangling bonds of the Si atoms along the steps. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1].

The long-range interaction of the two-fold and three-fold periodicity is investigated by spot-profile analysis in LEED at a sample temperature of 80 K. The strict two-fold periodicity of the Au atoms is not correlated between adjacent wires as concluded from the streak like intensity in LEED. In contrast, the threefold ordering of the Si spins exhibit a clear ordering perpendicular to the Au wires. A modification of the structure model [2] explains the structural correlation between adjacent Si step edge atoms. The resulting frustrated structure indicates the formation of a 2D spin-liquid in this system [2].

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32. Ultrafast non-thermal switching of a surface CDW system in the regime of critical damping

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The wire-type arrangement of Indium atoms on a Silicon(111) surface serves as a famous prototype for the formation of a (quasi-)one-dimensional charge density wave (CDW) groundstate. At room temperature, the indium atoms are arranged in parallel zig-zag chains, forming a metallic (4×1) structure. Cooling the system down below a critical temperature of T_c = 130 K leads to a structural phase transition: the indium atoms rearrange to hexagons, the periodicity doubles and an (8×2) reconstructed groundstate occurs. The structural transition is accompanied by a metal-to-insulator transition (MIT) through the opening of a bandgap in the electronic structure of about 100 meV.
Ultrafast time-resolved electron diffraction was used to investigate the transient non-equilibrium structural dynamics of the (8×2) → (4×1) phase transition. In this pump-probe setup the sample is excited with 80 fs laser pulses at a peak wavelength of 800 nm and probed with sub-300 fs electron pulses in a surface sensitive geometry, i.e., under reflection at grazing incidence angles of 1° to 6°. Utilizing a tilting pulse front scheme we improved the overall temporal resolution of this setup to less than 350 fs.
Excitation of the (8×2) groundstate with fs-laser pulses revealed the existence of a metastable (4×1) phase. This supercooled phase survives for hundreds of picoseconds due to an energy barrier of 40 meV. However, at fluences of 7 mJ/cm² the CDW groundstate is lifted across the entire surface within 350 fs. A transient temperature rise of the Indium layer was determined through the intensity of the thermal diffuse background utilizing the Debye-Waller effect. The laser induced heating by less than 80 K takes place on timescales 6 times slower than the MIT, which clearly rules out a simple thermal excitation scenario of the phase transition. Instead, we explain the observed dynamics through a displacive excitation scenario, where the optical excitation of the electronic subsystem modifies the potential energy surface of the system. What follows is the accelerated cooperative motion of the surface atoms into the energetically favored (4×1) phase. The phase transition time scales exponentially with the number of excited electrons, i.e. with the laser fluence. Recent DFT calculations (A. Lücke, W.G. Schmidt, Uni Paderborn) confirm this scenario and show that certain electronic states have to be occupied to excite the relevant phonon modes which drive the structural transformation within $1/4^{th}$ of a soft mode period.
In contrast to many other CDW systems, the observed structural transition occurs without any sign of an oscillatory behavior. This is explained through a strong coupling of the In atoms to the substrate which facilitates the sub-ps structural response by a rapid dephasing and damping of the two characteristic phonon modes. The transition thus proceeds in the limit of critical damping and cannot be faster than in this limit.

33. Epitaxial Sn on h-BN terminated ZrB_2

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Stanene, the tin analogue of graphene, promises a wealth of physical phenomena and bright perspectives for electronic applications. Due to its strong spin orbit coupling (SOC), the quantum spin Hall insulator phase is expected to exist even at room temperature. Epitaxial stanene, exhibiting a buckled honeycomb Sn-lattice, has been prepared so far on only one substrate - Bi_2Te_3. Because of the interaction with the substrate, the electronic structure of the epitaxial stanene does not correspond to that of theoretically predicted free-standing stanene. This warrants studies of Sn-lattices on weakly interacting, preferably electrically insulating, substrates.
We found that after depositing a sub-monolayer of Sn on a h-BN terminated ZrB_2 thin film [1-3] and subsequent annealing at 670˚C, we could observe a new surface reconstruction (see Fig. 1 and Fig. 2). The Sn LEED pattern matches the ZrB_2(4x4) and h-BN(5x5) patterns and we suspect a Sn(3x3) reconstruction. The estimated Sn lattice parameter of 4.2Å is significantly different from free-standing stanene, such that the ordered Sn phase we observe could be due to a different lattice with hexagonal symmetry. Further investigations of the structural and electronic properties of this novel Sn layer are ongoing.

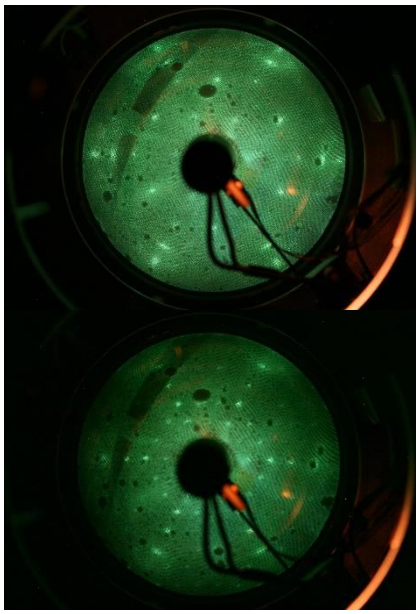

Fig. 1: LEED image at 85eV of pristine h-BN/ZrB_2 sample(up) and after Sn deposition and annealing at 670°C(bottom). Additional LEED spots emerge.

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