Schloss Ringberg

Symposium



Tegernsee

17-20 February 2019

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Publisher:

Christoph Tegenkamp, Institut für Physik, TU Chemnitz, 09126 Chemnitz Martin Wolf, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin

Venue: Tagungsstätte Schloss Ringerg, Schloßstrasse 20, 83708 Kreuth

Coffee breaks & Meals

- Breakfast in the castle is served 8:00 9:00. Breakfast times in the hotel "Zur Post" are 7:00 10:00.
- Lunch is served every day at 12:30 13:30.
- There is a coffee break in the morning and one in the afternoon. The times are listed in the program.

Internet access at the venue

To access the wireless LAN service, please use the following password: 170219fk

Music program

The following compositions will be played live by Jusara Moser (Bassoon, Piano), Claudia Pfnür (Viola) and Herbert Pfnür (Violoncello) after the laudatio and during the "Bayerischer Abend" on Tuesday, February 19, 2019.

- Wolfgang Amadeus Mozart (1756 1791): Duet for Bassoon and Violoncello KV 292 Allegro - Andante - Allegro
- Alessandro Rolla (1757 1841): Duet for Viola and Violoncello Andantino - Largo apassionato - Rondo allegretto
- Johannes Brahms (1833 1897): Trio for Piano, Viola and Violoncello op. 114 Allegro - Adagio - Andantino grazioso – Allegro

Venue and emergency number

SCHLOSS RINGBERG Tagungsstätte der Max-Planck-Gesellschaft Schlossstr. 20 83708 Kreuth

emergency No. 🕾 +49 (0)176-28371883 (Christoph Tegenkamp, mobile)

Program Overview

Monday, 18 February 2019

9:00-9:10		Opening remarks	
9:10-9:45	К1	Franz Himpsel	Electronic properties of atomic wires: from semiconductor surfaces to organic chains and DNA
9:45-10:15	11	Ulrich Köhler	Low-dimensional nanostructures on compound semiconductors: structure, magnetic properties and substrate-island interaction
10:15-10:45	12	Dietrich Zahn	Enhanced Raman Spectroscopy of Low-dimensional Semiconductor Structures
10:45:11:15		Coffee break	
11:15-11:50	К2	Ulrich Höfer	Ultrafast Time-Resolved Investigations of Electron Transport at Surfaces and Internal Interfaces
11:50-12:20	13	Hugo Dil	Electronic structure of polar and ferroic surfaces
12:30:13:30		Lunch	
13:30-14:05	КЗ	Ralph Claessen	Local spectroscopy of helical 1D edge states in a quantum spin Hall insulator
14:05-14:35	14	Harold Zandvliet	Charge puddles in germanene
14:35-15:05	15	Manuel Ligges	Time-domain observation of femtosecond hot carrier transport in nanostructures
15:05-15:35	16	Martin Weinelt	Electron dynamics in spin-orbit materials
15:35-16:15		Coffee break	
16:15-16:50	17	Herbert Pfnür	How 1D are atomic wires? Promises and perspectives
17:00-18:00		Guided tour / Ringber	rg castle
18:30-19:15		Dinner	
19:15	Р	Poster session / Research Unit 1700	

Tuesday, 19 February 2019

9:00-9:35	К4	Silke Biermann	Correlated electron materials a playground for theoreticians
9:35-10:05	18	Wolf Gero Schmidt	Coupling of electronic and atomic degrees of freedom in quasi-1D systems from first-principles calculations
10:05-10:35	19	Friedhelm Bechstedt	Quantum spin Hall phase versus quantized spin Hall conductivity?"
10:35-11:00		Coffee break	
11:00-11:30	I10	Volkmar Zielasek	Two routes off the beaten track towards metal nanoparticle catalysts
11:30-12:00	111	Meyer zu Heringdorf	Surface Plasmon Vortex Focussing
12:00-12:30	112	Mario Rocca	Conventional and acoustic surface plasmon dispersion at metal surfaces: an overview on High Resolution Electron Energy Loss investigations
12:30:13:30		Lunch	
13:30-17:00		Excursion	
17:30-18:10		Michael Horn von Hoegen	Laudatio + Musical accompaniment
Following this		Bayerischer Abend	

Excursion:

We offer two different kind of excursions. Depending on your registration you can attend a guided hiking tour or a sledge ride at Wallberg (https://www.wallbergbahn.de/winter/die-rodelbahn/).

Wednesday 20 February 2019

9:00-9:35	К5	Hanno Weitering	Potential for high-temperature superconductivity on a silicon platform
9:35-10:05	113	Stefan Fölsch	Quantum dots and quantum rings engineered by atom manipulation
10:05-10:35	114	Jörg Kröger	Spectroscopy of currents and forces in scanning probe junctions
10:35-11:00 Coffee break		Coffee break	
11:00-11:30	115	Moritz Sokolowski	Organic Molecules observed on Flatland by Optical Spectrosopy
11:30-12:00	116	Michael Tringides	Metal growth on and under graphene: intercalation, novel 2-d phases and heterostructures
12:00-12:30	117	Wolf Widdra	History and Future of Surface Quasicrystallography
12:30		Closing remarks	
12:30-13:00		Lunch	
13:00		Departure	

Keynote talks

Electronic Properties of Atomic Wires: from Semiconductor Surfaces to Organic Chains and DNA

F. J. Himpsel

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Low-dimensional solids exhibit strange new phenomena, such as fractional statistics in 2D (anyons) and the transformation of nearly-free electrons in 3D metals to highly-correlated objects in 1D (spinons and holons). Electrons interact strongly in 1D, because they cannot avoid each other when traveling along the same quantum wire. Such wires can now be fabricated with atomic precision by several techniques, for example by self-assembly of metal atoms at stepped semiconductor surfaces, by atom manipulation in a low-temperature STM, or by synthesis of tailored DNA oligomers. Such structures serve as prototypes for testing the quantum limits of electronics. Various phenomena and concepts of low-dimensional physics will be introduced, including popular terminology borrowed from particle physics, such as "Dirac cone", Weyl fermion, and Majorana particle.

Ultrafast Time-Resolved Investigations of Electron Transport at Surfaces and Internal Interfaces

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Time-resolved photoelectron spectroscopy, a method that combines femtosecond pump-probe techniques with angle-resolved photoelectron spectroscopy (ARPES), can be used to perform measurements of electron transport at interfaces in a contact-free fashion and with femtosecond time-resolution. In a first example, I will discuss results obtained for well-defined model systems of organic/metal contacts. The experiments show that interface-specific electronic states efficiently mediate the electron transfer between metals and organic semiconductors. In a second example, I will discuss Dirac surface states of topological insulators. We induce electrical currents in these states with strong THz transients and directly access their dynamics in momentum space with subcycle time resolution (Fig 1). As a result of spin-momentum locking, the accelerated spin-polarized electrons reach ballistic mean free paths of several hundreds of nanometers. Topological insulators are thus promising materials for future lightwave-driven electronics operating at THz clock rates.



Fig 1: a Scheme of the THz-ARPES experiment at Bi_2Te_3 : Electrons in the topological surface state are accelerated by a linearly polarized THz field E_{THz} (red and blue waveforms) and photoemitted by a time-delayed ultrashort UV pulse (violet). **b-d** Photoemission maps: Before the arrival of the THz field (**b**), right after the positive field crest (**c**) and just after the negative field maximum (**d**). The electron distribution is accelerated away from the Fermi level (white-dashed line) and shifted along the V-shaped dispersion of the topological surface band. **e** Temporal evolution of the current density extracted from the photoemission maps (data points) as comparted to the E_{THz} (black dashed line) and the results of simulations using scattering times of 1 ps (red solid curve). [adopted from Reimann *et al.*, Nature **562**, 396 (2018)].

Local spectroscopy of helical 1D edge states in a quantum spin Hall insulator

K3

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Two-dimensional topological insulators are characterized by hosting spin-polarized conducting band states at their one-dimensional (1D) edges. These edge states are spin-momentum locked and hence protected against single-particle backscattering, leading to the quantum spin Hall (QSH) effect. In contrast, topological protection does not impede *two-particle* scattering caused by electron-electron interaction, and therefore the 1D edge states are in principle expected to form a (helical) Tomonaga-Luttinger liquid (TLL). So far, however, there has been no clear experimental evidence to verify this conjecture.

Recently, we succeeded in synthesizing bismuthene, i.e., a monolayer honeycomb lattice of Bi-atoms, on a SiC(0001) substrate [1], which according to density functional theory is a QSH insulator with a bulk band gap of ~0.8 eV [2]. Due to this large gap the topological edge states are laterally confined to almost atomic dimensions, making their spatial identification directly accessible to scanning tunneling microscopy and spectroscopy (STM/STS). We will discuss especially the local density of states measured by STS at the 1D edges which displays all fingerprints of TLL behavior, thereby providing the first such spectroscopic identification in a QSH insulator [3]. Finally, we will discuss how the topological protection can be switched off when bringing two edges into close contact, e.g., at phase slip domain boundaries of the $\sqrt{3} \times \sqrt{3}$ bismuthene reconstruction on the SiC substrate, giving rise to the formation of Fabry-Perot-like quantum well states between neighboring scattering centers.



Fig. 1: STM topography of bismuthene/SiC(0001) (left) and universal scaling of the STS edge state spectra (right).

- [1] F. Reis et al. Science 357, 287 (2017).
- [2] G. Li et al. Phys. Rev. B 98, 165146 (2018).
- [3] R. Stühler et al. submitted.

Correlated Electron Materials – a Playground for Theoreticians

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Spectroscopic techniques are the first choice for characterizing the electronic structure of materials. In materials with strong electronic Coulomb correlations, however, spectral functions thus measured can be far from a simple single-particle band picture.

In this talk, we will first review basic concepts of electronic correlations and their modelisation [1], with examples taken among transition metal compounds [2-5] and f-electron systems [6,7]. We will then discuss the current state-of-the-art of electronic structure calculations for correlated materials, as well as open questions and further perspectives in the field.



Fig1: Spectral function of Sr2IrO4 (constant energy cuts) from angle-resolved photoemission spectroscopy (left) and combined density functional dynamical mean field theory calculations (right). From [4].

[1] S. Biermann, Review article in: First principles approaches to spectroscopic properties of complex materials,

Topics in Current Chemistry, edited by S. Botti, M. Cococcioni, C. Di Valentin, Springer, 2014.

[2] C. Martins, L. Vaugier, M. Aichhorn, S. Biermann, Phys. Rev. Lett. 107 266404 (2011).

[3] C. Martins, M. Aichhorn, S. Biermann, J. Phys.: Condens. Matter 29 263001 (2017)

[4] C. Martins, B. Lenz, L. Perfetti, V. Brouet, F. Bertrand, S. Biermann, *Phys. Rev. Materials* 2, 032001 (Rapid) (2018)

[5] B. Lenz, C. Martins, S. Biermann, submitted to J. Phys. Condens. Matter (2018).

[6] J.M. Tomczak, L.V. Pourovskii, L. Vaugier, A. Georges, S. Biermann, Proc. Nat. Ac. Sc. USA 110 (3) 799 (2013).

[7] Pascal Delange, Silke Biermann, Takashi Miyake, Leonid Pourovskii, Phys. Rev. B 96, 155132 (2017).

Potential for unconventional superconductivity on a silicon platform

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The rich physics of doped Mott insulators is at the heart of high-temperature superconductivity in complex oxide compounds, although the precise mechanism for high temperature superconductivity is still up for debate. Advances in this field would greatly benefit from the availability of new material systems with similar richness of physical phenomena, ideally those that are much less complex in structure and composition, and easier to model theoretically. Here we show that such a system could potentially be realized on a silicon surface [1]. Adsorption of one-third monolayer of Sn atoms on a Si(111) surface produces a triangular surface lattice with half-filled dangling bonds. Modulation hole-doping of these dangling bonds unveils clear hallmarks of Mott physics, and additionally produces a sharp 'van Hove' singularity in the density of states just below the Fermi level. At a critical doping level, we observe a strong zero-bias anomaly in the local density of states, possibly signaling the formation of a magnetic or superconducting gap [2]. These observations are remarkably similar to those made in complex oxide materials, including the high-temperature superconductors, but highly extraordinary within the realm of conventional *sp*-bonded semiconductor materials. They suggest that exotic quantum matter phases could possibly be realized and engineered on silicon-based materials platforms.

[1] F. Ming et al. *Phys. Rev. Lett.*, **119**, 266802 (2017).

[2] F. Ming et al., *Phys. Rev. B* 97, 075403 (2018)

Invited talks

Low-dimensional nanostructures on compound semiconductors: structure, magnetic properties and substrate-island interaction

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Nanometer scale layers and particles on semiconducting or insulating substrates are widely used for scientific or technological applications. Low dimensional magnetic structures on compound semiconductors are useful spin injection experiments. Here the understanding of the correlation between structure and magnetism is essential for the optimization of the deposition of ferromagnetic structures on semiconductors functional as spin injectors.

Elemental ferromagnets like nickel or iron provide a high Curie temperature but a bad lattice fit to GaAs and InAs. The system Fe₃Si/GaAs is a FM/SC combination that possesses properties such as a low lattice mismatch, high Curie temperature, high thermal stability and halfmetallic behavior that make it an interesting candidate for spintronic devices. From in-situ MOKE, SQUID and FMR measurements the magnetic moments as well as the magnetic anisotropies can be determined as a function of the layer thickness and are correlated with the structural information determined by STM. In the low coverage regime magnetically and structurally independent Fe₃Si-island lead to a super-paramagnetic behavior at room temperature (see left side of Fig. 1) which switches to a ferromagnetic behavior above 3ML.

Sb-based halbmetallic structures on GaAs like CrSb or MnSb which provide other possibilities to fabricate zero-dimensional structures will be discussed.

Nanometer-scale metallic clusters on semiconducting oxides are useful for applications in catalysis. For the system copper on ZnO it will be shown that using STM-tip manipulation one can obtain information on the interface between the substrate and the nano-cluster (see right side of Fig. 1).





Fig.1: left: SQUID field-cooled, zero-field-cooled curves of a Fe₃Si/GaAs layer, inset: morphology of the layer right: "footprint" of a Cu-island on ZnO after removal using the STM-tip

Enhanced Raman Spectroscopy of Low-dimensional Semiconductor Structures Dietrich RT Zahn¹, Volodymyr Dzhagan², Alexander Milekhin³

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The ever decreasing dimensions of components in (opto-)electronic devices towards the nanometer scale clearly reveals the need for optical spectroscopies to be sensitive to ultra-small amounts of matter as well as break the diffraction limit of light in order to achieve ultra-high lateral resolution. Raman spectroscopy is a widely used optical spectroscopy as it provides a vast amount of information including *e.g.* composition, strain, crystal structure, and crystallinity.

Here we will first review techniques to enhance the Raman signals of very small amounts of material. One important ingredient of enhancing Raman signals is employing resonance excitation, *i.e.* choosing the exciting laser photon energy so that it coincides with a maximum in optical absorption. Often resonance enhancement alone is not sufficient when the amount of matter is very small, for instance for detecting the Raman spectrum of a few or even a single nanostructure. Then further enhancement strategies need to be engaged such as surface-enhanced Raman spectroscopy (SERS). In the case of SERS manifold realisations using ordered nanostructured surfaces with various metals have been applied. The metallic nanostructures can be prepared by expensive techniques such as electron beam lithography or less expensive ones such as nanosphere lithography.

The last part will be devoted to achieving lateral resolution on the nanoscale using tip-enhanced Raman spectroscopy (TERS). The technique requires the combination of a Raman spectrometer and an atomic force microscope using a conductive tip for the plasmonic enhancement so that the lateral resolution is determined by the tip radius. Giant enhancement is observed when detecting the Raman spectra of materials in the plasmonic gap between the metallic tip and metallic nanostructures. Finally the detection of the Raman spectrum of a single semiconductor quantum dot is demonstrated.

Electronic structure of polar and ferroic surfaces

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Polar charge order has a strong influence on the electronic structure of materials and has experienced a revived interest in recent years. The symmetry breaking in ionic materials and resultant electric field lead to a strongly enhanced Rashba-type spin orbit splitting in bulk materials [1,2] and Wannier-Stark localization of free electrons [3]. At surfaces and interfaces the additional degree of freedom can lead to spontaneous polar order in non-polar materials, which in turn can lead to the formation of a 2DEG at the surface or interface [4]. Combined with correlation effects and magnetic order [5] this provides a rich phase diagram for the creation of emerging systems with novel electronic properties.

In this work (spin- and) angle resolved photoemission (S)ARPES will be used to show how the spin and electronic structure of such states can be tuned to achieve the required properties. By using the first *operando* SARPES measurements the reversal of the spin texture in a ferroelectric by an external electric field will be demonstrated [6]. In similar experiments on a multiferroic system the strong magnetoelectric coupling allows to switch the magnetic order by an electric field, whereby the complex switching pathway can be deduced from the spin texture.

For the surface 2DEG on titanates, and especially $SrTiO_3(001)$, it will be shown how typical surface science approaches can be used to manipulate the spin texture and electronic structure, thereby again establishing that the origin of the 2DEG lies in structural distortions [7]. Furthermore, because of the peculiar polaronic properties of the material also a change in dielectric response has a direct influence on the structural relaxation and therefore the electronic structure of the 2DEG [8].

- [1] G. Landolt et al. Physical Review Letters 109, 116403 (2012).
- [2] J. Krempasky et al. Physical Review B 94, 205111 (2016)
- [3] S. Muff et al. Physical Review B 98, 045132 (2018)
- [4] M. Setvin et al. Science 359, 572 (2018)
- [5] A. Santander-Syro et al. Nature Materials, 13, 1085 (2014)
- [6] J. Krempasky et al. Physical Review X 8, 021067 (2018)
- [7] M. Radovic et al. (in preparation)
- [8] E. Bonini Guedes et al. (in preparation)

Charge Puddles in Germanene

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We have investigated the structural and electronic properties of germanene, the graphene-like allotrope of germanium, grown on a molybdenum disulfide (MoS₂) substrate. The deposited germanium atoms nucleate at pre-existing defects in the MoS₂ substrate and form two-dimensional germanene islands with a lattice constant of 3.8 Å and a height of 3.2 Å. Scanning tunneling spectroscopy measurements recorded on the germanene layer reveals a V-shaped density of states, which is one of the hallmarks of a two-dimensional Dirac material. We have recorded spatial maps of the minimum of the differential conductivity, also referred to as the charge neutrality or Dirac point. The Dirac point maps reveal the presence of well-defined charge puddles in the germanene sheet. The Dirac point varies from -30 meV to +15 meV, corresponding to a charge density in the puddles in the range of 2.6×10^{-3} electrons to 6.6×10^{-4} holes per nm². The radius of these puddles is about 10-20 nm, resulting in a total charge of the order of one charge carrier per puddle. The defect concentration in the top layer of the MoS₂ substrate is very comparable to the density of charge puddles, suggesting that the charge puddles are caused by the charged defects in the top layer of the MoS₂ substrate.

Time-domain observation of femtosecond hot carrier transport in nanostructures

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Analysis of the electronic structure of solid matter is widely based on angle-resolved photoemission spectroscopy (ARPES), which is a surface sensitive technique due to the short inelastic mean free path of photoelectrons of several 10 eV kinetic energy. An extension towards bulk sensitivity is in principle possible by a considerable in- or decrease of the kinetic energy in hard X-ray photoelectron spectroscopy (HAXPES) or Laser-based ARPES, respectively. All these techniques analyze mainly the electronic structure $E(\vec{k})$. Of similar interest are dynamic properties like, e.g. the energy- and momentum-dependent velocity of electrons $v_g(E) = \hbar^{-1} \vec{\nabla}_{\vec{k}} E(\vec{k})$, which can be determined using femtosecond time-resolved, non-linear photoelectron spectroscopy, as demonstrated here.

Using a back-pump/front-probe geometry (Fig1), we analyze bulk-like transport properties through time-of flight measurements of photoexcited electrons in nanometer thin, epitaxially grown Au/Fe/MgO(001) multilayer samples. This sample geometry was chosen as it restricts the optical excitation to the Fe-layer, leading to a well-defined spatial excitation profile. For photoexcited electrons in the energetic range $E-E_F=0.7-1.0$ eV, we find that the arrival times of Fe back-pumped electrons on the Au front surface depends linearly on the Au film thickness (5-30 nm). Numerical and analytical solutions of the linear transport equation, including inelastic population decay, indeed shows that such a behavior is expected for ballistic electron transport. The extracted energy-dependent ballistic velocities slightly increase with energy and are found to be in good agreement with previously reported (energy- and *k*-averaged) values of $v_{AU} \sim 0.9-1.4$ nm/fs [2-4]. The establishment of this technique allows for future studies of more complex materials in which the exact role of charge transport or transfer is under debate.



Fig1: Back-pump/front-probe scheme. Electrons are excited by a femtosecond laser pulse ($\hbar\omega$ =2.0 eV) in the Fe injection layer and probed by photoemission ($\hbar\omega$ =3.9 eV) after their propagation through Au layers of different thickness.

This work is supported by the Deutsche Forschungsgemeinschaft through the collaborative research center SFB1242.

- [1] see, e.g. M. Bauer et al. Prog. Surf. Sci., 90, 319 (2015).
- [2] S.D. Brorson et al. Phys. Rev. Lett., 59, 1962 (1987).

[4] A. Melnikov et al. Phys. Rev. Lett., 107, 076601 (2011).

^[3] T. Juhasz et al. *Phys. Rev B*, **48**, 15488 (1993).

Electron dynamics in spin-orbit materials

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Topological insulators (TIs) host metallic topological surface states with helical spin structure. This makes them promising materials for the generation of spin-polarized currents. The TI Bi₂Se₃ is intrinsically n-doped and exhibits an occupied and an unoccupied topological surface states at the Γ point with a Dirac cone dispersion.

It has been disputed, whether photocurrents, induced in Bi₂Se₃ with circularly polarized light stem from these Dirac cones. We studied the momentum distribution of electrons excited with circularly polarized light from the first into the second Dirac cone of Bi₂Se₃ with two-photon photoemission and one-step photoemission calculations.

We find dichroic photoemission for circularly polarized pump pulses, both at resonant and offresonant excitation. While a two-dimensional (E,k_y) -cut perpendicular to the plane of incidence would support the commonly assumed coupling of the photon angular momentum to the electron spin, it is inconsistent with the observed azimuthal (k_x, k_y) – patterns. Instead it reflects the surface point group. The only twofold-symmetric patterns appear in the energy range, in which surface and bulk states hybridize. In general, a threefold-symmetric dichroic signal does not support unidirectional photocurrents. Nevertheless, the residual asymmetry of up to 3.5% in our photoemission spectra is compatible with previously observed helicity-dependent photocurrents.

BiTeI is a layered semiconductor without inversion symmetry. Strong spin-orbit coupling leads to a giant Rashba-splitting of the BiTeI surface and bulk bands. Crystalline BiTeI is known to cleave along the van-der-Waals-bonded layers of Te and I. This results in either Te- or I-terminated surfaces depending on the orientation of the crystal.

We studied the population dynamics of excited carriers in pure and Mn-doped BiTeI. Applying a 6.2-eV probe pulse, we monitor the Rashba-split surface state and conduction band on the Teterminated surface. Its surface state has a nearly isotropic free-electron-like dispersion with a positive effective mass. Excitation with a 1.5-eV pump pulse generates hot electrons with picosecond decay times. The lifetimes of electrons do not depend on the sample temperature (50 vs 300 K). In contrast, we find a very different behavior for hole lifetimes. They are rather constant, overall smaller than corresponding electron lifetimes, and show a strong temperature dependence.

We attribute this behavior to the opening of an additional plasmon-emission channel.

*This work results from collaborations between groups at FU Berlin¹, FAU Erlangen², LMU München³, St. Petersburg State University⁴, Novosibirsk State University⁵ and Tomsk State University⁶.

¹ Sophia Ketterl, Marco Polverigiani, Martin Bastian, Cornelius Gahl, Beatrice Andres ² Sebastian Otto and Thomas Fauster, ³ Jürgen Braun, Jan Minar, and Hubert Ebert, ⁴ Vladimir Voroshnin and Alexander Shikin, ⁵ O. E. Tereshchenko, ⁶K. A. Kokh.

How 1D are atomic wires? Promises and perspectives

Herbert Pfnür

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Coupling of quasi-one-dimensional systems to a substrate turned out to reveal a rich variety of new physics and to be full of complexity. This is even true for the relatively simple case of semiconductor surfaces of (stepped) Si and Ge, in which the electronic decoration and modification of surface states mostly determine the physical properties of the whole now quasi-1D systems. They can thus be considered to be prototype examples. Even in these systems neither the formation of even single atomic chains nor the appearance of a quasi-1D Fermi surface are sufficient for the classification as a quasi-1D system, as will be shown. It seems more that the occuring phase transitions (or their absence) are better indicators. While the "classical" 1D instabilities such as Peierls, CDW, SDW, superconductivity etc. partly still appear, they are strongly modified or are even replaced by new types of phase transitions due to electronic hybridization in more than 1D and to new electronic correlations, leading, e.g. to metallicity at low temperatures. Several characteristic examples will be discussed. Embedding into 3D, though some promising first results exist, is still a largely unsolved problem.

Coupling of electronic and atomic degrees of freedom in quasi-1D systems from first-principles calculations

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Minute structural changes may lead to drastic modifications of the electronic properties of quasi-1D systems, while, on the other hand, an electronic charge redistribution, induced, e.g. by optical excitation may induce pronounced structural modifications in such systems. This is illustrated in my talk using two prominent examples: (i) Localized photoholes at the Brillouin zone boundary of the In/Si(111)(8x2) nanowire system are shown to drive an ultrafast (8x2) \rightarrow (4x1) phase transitions that is accompanied by the formation of metallic In-In bonds along the wire direction [1,2]. (ii) A $sp^3 \rightarrow sp^2+p$ rehybridization accompanied by a lateral surface charge transfer is demonstrated to destabilize the Si(553)-Au spin chains [3] with respect to a diamagnetic surface that complies with electron counting heuristics [4].



Figure: Calculated charge density redistribution due to the optical excitation of the In/Si(111)(8x2) surface. Photoholes (red) reduce the strengths of outer In-In dimer bonds while charge accumulation (blue) enhances the diagonal bond across the In hexagon. This results in a (8x2) \rightarrow (4x1) phase change.

[1] T Frigge, B Hafke, T Witte, B Krenzer, C Streubühr, A Samad Syed, V Miksic Trontl, I Avigo, P Zhou, M Ligges, D von der Linde, U Bovensiepen, M Horn-von Hoegen, S Wippermann, A Lücke, S Sanna, U Gerstmann, WG Schmidt,

Nature 544, 207 (2017).

[2] CW Nicholson, A Lücke, WG Schmidt, M Puppin, L Rettig, R Ernstorfer, M Wolf, Science 362, 821 (2018).

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Quantum spin Hall phase versus quantized spin Hall conductivity?

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The quantum spin Hall (QSH) phase is a quantum state of matter, proposed to exist in twodimensional (2D) semiconductors with inverted band structure and, hence, a character of a topological insulator (TI). Such a quantum phase should exhibit a spin Hall (SH) conductance but a vanishing charge Hall conductance. Since no external magnetic field is present, it can only be realized in materials with strong spin-orbit interaction (SOI). As central questions we investigate if the QSH phase is indeed characterized by a quantized static SH conductivity and how the answer depends on translational and point-group symmetry.

As central quantities we study the SH conductivity $\sigma_{xy}(\omega)$ via the Kubo formula [1] and the Z₂ topological invariant via the parity method [2] by means of *ab initio* calculations of relativistic electronic structures of infinite 2D sheet crystals. Besides the dynamical quantity, the third-rank tensor of the static SH conductivity is computed for three Z₂=1 classes: Hexagonal honeycomb atomic layers made by group-IV elements, germanene (Ge) and stanene (Sn), and their chemically functionalized, e.g. hydrogenated (GeH), iodinated (GeI) or fluoroinated (SnF), counterparts [3]. Square and rectangular 2D Bravais lattices are viewed for the model systems 1S- and 1T'-MoS₂ as well as -WS₂. In addition, dynamical results are given for atomically thin Ge-based systems [3]. The influence of destroying the inversion symmetry, e.g. by vertical electric fields, is discussed.

The inverted band structures with a fundamental gap due to SOI are strongly modified by functionalization with I, F or H. As a consequence, we observe drastic changes in the frequency dependence of $\sigma_{xs}(t_{0})$. For hexagonal 2D TIs the static SH conductivity for z-spin orientation exhibits quantization with e^2/h , the reciprocal von Klitzing constant, as shown in Fig. 1 [1,3]. This value is hardly influenced by temperature or Fermi level position. While for 2D square 1S crystals the quantization is less destroyed, the conductivity value tends to zero for rectangular 1T' systems. Lifting the inversion symmetry, the quantization is violated also for hexagonal sheets. We conclude that the QSH phase is not generally characterized by a quantized SH conductivity, only for high-symmetric cases.



Fig. 1: Real (solid) and imaginary (dashed) part of spin Hall conductivity for Ge, GeI and GeH. Red circles indicate quantization.

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Two routes off the beaten track towards metal nanoparticle catalysts

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Many solid catalysts in industrial applications are highly dispersed metal nanoparticles on carbon or oxide supports. Commonly, such catalysts are prepared from liquid solutions of a metal precursor via impregnation or precipitation directly on or together with the support. Thereby, nanoparticle size, shape, composition (in case of bimetallic precursors), and distribution - all relevant for catalytic performance - are typically poorly controlled.

Colloidal chemistry has advanced to produce, bottom-up and without the need for any solid support, stocks of nanoparticles of tunable and uniform size, shape, composition, and surface termination for a wide range of metals. Two recent and particular routes towards metal nanoparticle catalysts based on colloidal chemistry will be presented:

I) Reverse block copolymer micelles have been employed as 'nanoreactors' for the production of bimetallic AgAu nanoparticles from metal salt solutions [1]. By adjusting metal salt loads and micelle core diameters, the particle size and composition can be tuned independently. Deposited on various oxide supports, these particles catalyze the oxidation of CO in air and reveal, as model catalysts, the dependence of catalytic activity on nanoparticle composition, size and support.

II) Stable, solid networks of organic ligand-linked Pt nanoparticles may be generated by mixing Pt colloids with solutions of bifunctional amine-terminated spacer molecules, both ends of which bind easily to Pt [2]. These networks exhibit a high density of Pt surface sites at low heat capacity which renders them ideal catalysts for catalytic sensing of combustible gases. Thermopile-based microsensors which detect the reaction heat generated during catalytic H₂ oxidation in air at ligand-linked Pt nanoparticle networks show excellent sensitivity, response time, and stability.



Fig1: p-phenylenediamine-linked Pt nanoparticles in TEM (left) and network concept (right).

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Surface Plasmon Vortex Focussing

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Surface plasmon polaritons (SPPs) are collective oscillations of electrons at an interface between a noble metal surface and a dielectric material. SPPs can be excited by light, and by using focused ion beam milling for structuring of grating couplers, it is possible to control the starting location of SPPs with sub-wavelength precision and thus manipulate the shape of SPP phase-fronts at the nanoscale. A normal-incidence time-resolved photoemission electron microscopy (PEEM) experiment with <15 fs short laser pulses produces a direct conceptual visualization of the excited fs SPP pulses [1] and provides for imaging of propagating and interfering SPP pulses in space and time [2]. In transient standing-wave SPP fields, an unexpected time-signature of the nonlinear photoemission yield is observed. By employing a transit-time separation of the exciting laser pulse from the SPP, the electron emission must be explained exclusively with the SPP field (plasmoemission) [3]. Using circular grating couplers, small SPP focus spots can be formed [4], from which highly nonlinear above threshold (plasmo)electron emission is observed. SPPs with angular orbital momentum [5] can create even stronger fields in a SPP focus. The analytical solutions for SPPs excited at an Archimedean spiral show that for a total angular momentum of J=0 a defined focus spot with a transverse SPP field is obtained [6]. In such focus spots, the plasmoemission mechanism is gradually driven into the strong-field regime.



Figure 1: Energy Spectrum of the spatial distribution of electrons, emitted from the focus spot of a SPP. The SPP was excited on a Au surface, using circularly polarized light with an Archimedean spiral grating coupler to yield a J=0 state. Maxima in the sections along the position axis show emission from the different anti-nodes of the formed SPP interference pattern. Sections along the energy axis show electron emission processes of higher orders. The highest nonlinearities are found in the center of the plot, where above threshold ionization of up to 6th order can be identified.

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Conventional and acoustic surface plasmon dispersion at metal surfaces: an overview on High Resolution Electron Energy Loss investigations

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Here I will give a summary of three decades of experimental investigations of collective electronic excitations at metal surfaces performed with high resolution electron energy loss spectroscopy, a technique which allows for a high resolution in reciprocal space when operated at grazing incidence (HREELS) or coupled with a SPA-LEED optics (ELS-LEED). The latter studies implied a fruitful collaboration between Genova and Hannover.

These investigations evidenced the negative (positive) dispersion of the ordinary surface plasmon on simple (noble) metal surfaces, a phenomenon caused by the increasing confinement in the near surface region of the electric potential associated with the induced charge with exchanged momentum. The very sharp surface plasmon loss of Ag allowed to evidence the anisotropy of the dispersion coefficient with respect to crystallographic face as well as direction, effects which were qualitatively described by a model treating the d-electrons as a polarizable effective dielectric medium. Further data, recorded for Pd(110), showed a strong negative dispersion of the plasmon, an effect so far not investigated by theory.

More recently, theory by the group of Donostia-San Sebastian, predicted the existence of the acoustic surface plasmon (ASP) associated with the excitation of surface Shockley states. In this case experiment followed theory, confirming the existence of the ASP for the closed packed surfaces of Be, Au and Cu. In the latter cases the loss falls inside the continuum of electron hole pairs, an effect explained only by more refined theory. Against expectation, no ASP was observed for Ag(111) for which very different energies are predicted by different theories. Moreover, no theory has been developed so far for the excitation of surface Shockley states located at the border rather than the centre of the two-dimensional Brillouin zone or for Tamm states. A loss with approximatively linear dispersion is indeed apparent in the HREEL spectra of Ag(100), however, at unexpectedly large energy loss values. Particularly intriguing is the investigation of the ASP for stepped surfaces since the ASP could then couple with light and be used in future ASP based devices. Only Au(788) has been explored so far. The current knowledge on Surface Plasmon Dispersion has been recently summarized in three chapters of the Springer Handbook of Surface Science which will, hopefully, appear soon [1].

 ^[1] Springer Handbook of Surface Science, eds. M. Rocca, T.S. Rahman, L. Vattuone Surface Plasmons and Plasmonics by M. Rocca Plasmons in one and two dimensions by H. Pfnuer, C. Tegenkamp, L. Vattuone Theory of electron energy loss and photoelectron spectroscopy of surfaces and to-dimensional crystals by V.M. Silkin, E.E. Krasovskii and V. U. Nazarov

Quantum dots and quantum rings engineered by atom manipulation

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Atom manipulation with the scanning tunneling microscope makes it possible to create ultimately small structures at surfaces. We extended this technique to III-V semiconductor surfaces and found that their electrostatic potential landscape can be designed by the controlled positioning of charged adatoms. In this way, quantum dots with identical, deterministic sizes can be created one atom at a time. By using the lattice of the InAs(111)A surface to define the allowed atomic positions, the shape and location of the dots is controlled with effectively zero error. The dots are assembled from +1 charged indium adatoms, leading to the confinement of intrinsic surface-state electrons. This approach enables one to construct quantum dots with a perfectly defined level structure, as well as dot assemblies whose quantum coupling has no intrinsic variation but can nonetheless be tuned over a wide range. In a very recent experiment, we constructed quantum rings which enable electron motion along a closed path without loss of phase coherence. Our data reveal the emergence of ringconfined states, specifically a single ground state with zero angular momentum and doubly degenerate excited states with non-zero angular momentum. This level structure can be modified by deliberate incorporation of point defects. The results discussed in this talk illustrate that atom manipulation in combination with scanning tunneling spectroscopy provides detailed insight into the quantumphysical properties of artificial surface structures at the smallest size scales. Understanding and controlling these properties – and the new kinds of behavior to which they can lead – will be crucial for integrating atomic scale devices with existing semiconductor technologies.

Spectroscopy of Currents and Forces in Scanning Probe Junctions

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The talk summarizes a few results that have recently been obtained by scanning tunnelling and atomic force microscopes. Rather than exposing every detail the presentation strives for taking a glimpse on aspects as diverse as the detection of photons emitted from single molecules, graphene phonon spectroscopy, the occurrence of Andreev reflection in single-molecule junctions, and the measurement of forces required to move single atoms on surfaces.

The spectroscopic line shape of fluorescence light emitted from a single hydrocarbon molecule unravels the interplay between the localized tip-induced plasmon, the inelastic tunnelling electron, and the molecular exciton [1].

Extraordinarily strong graphene phonon signals are observed for graphene-covered metal surfaces intercalated by alkali metals. They are theoretically described by appropriately considering the graphene-tip and graphene-substrate hybridization [2].

The gradual transformation of the Bardeen-Cooper-Schrieffer energy gap to a zero-bias resonance in spectra of the differential conductance of single- C_{60} junctions on a conventional superconductor reflects the transition from quasi-particle tunnelling to Andreev reflection [3]. The C_{60} orientation leaves its fingerprint in the Andreev reflection.

Force spectroscopy indicates that the lateral force required to move single adsorbed atoms on a superconductor does not depend on the superconducting state [4], which is suppressed by crossing the critical temperature and the critical magnetic field.

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Organic Molecules observed on Flatland by Optical Spectrosopy

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The adsorption of large π -conjugated organic molecules on well-defined surfaces has been a topic of large interest during the last years, because the surface has significant impact on their structural ordering and their electronic excitations. Here, optical spectroscopy is a very valuable method, although it is not very commonly used in surface science, yet. We will report on two topics related to the optical transitions of molecules on surfaces that were investigated by high resolution laser spectroscopy [1, 2].

The first topic, concerns the self-organization of molecules on surfaces which can lead to well-defined *two-dimensional* ordered molecular aggregates that are different to those known for the respective 3D-bulk materials. Thus, the intermolecular delocalization of the excitation can lead to new interesting optical phenomena present in bulk materials [3].

Further, we report on the detection of single molecules on surfaces by fluorescence excitation spectroscopy. As illustrated in Fig. 1 below, it is possible to separate the excitations of single molecules in the frequency range using the high resolution of laser spectroscopy. This yields insight inro the interactions of the molecules with their individual local environment on the surface [4].



Fig1: Fluorescence excitation spectra of PTCDA at KCl step sites measured at 6 K. a) Low resolution scan of the inhomogeneously broadened 0-0 transition. The measured profile shows a slight peak splitting at the top that can be explained by a superposition of the contributions of two different adsorption sites, the *deep vacancy site* and the *deep vacancy site* +1. The profile be fitted by two Lorentzian can contributions. Real space models of the two adsorption sites are given as an inset. b) High resolution scan in the low energy wing of the inhomogeneously broadened profile. The scans show the statistical fine structure with distinct maxima and minima fixed in position. The single peaks are the resolved zero phonon lines of single molecules.

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Metal growth on and under graphene:growth morphology and intercalation

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Graphene based electronic and spintronic devices require understanding the growth of metals on graphene. Several metals (Gd, Dy, Eu, Fe,Pb) deposited on epitaxial graphene were studied with STM, SPA-LEED and DFT. For practically all metals the growth mode is 3-d[1,2]. This is a result of the low ratio of the metal adsorption to metal cohesive energy and repulsive interactions between unscreened charges at the metal-graphene interface that favor islands of small "footprint". It is an open challenge to find ways to modify the growth to layer–by–layer for high quality metal contacts and graphene applications as a spin filter. By growing Dy at low temperatures or high flux rates it is found that upward adatom transfer is kinetically suppressed and layer-by-layer is possible[3]. These results are also relevant for metal growth on other 2-d van der Vaals materials that also have weak bonding with metals and favor 3-d metal growth.

The graphene-metal interaction is also important for metal intercalation which provides a novel way to tune graphene's properties, besides doping. However many issues related to the intercalation process itself are poorly understood, i.e., the temperature and entry points where atoms move below graphene, different intercalation phases, their coverage, etc. SPA-LEED and STM were used to study these questions for Dy intercalation. Spot profiles of several spots (specular, 6sq(3), graphene) are studied as function of temperature and electron energy to deduce the kinetics of intercalation and the layer where the intercalated atoms reside.

Dy nucleation experiments were performed on graphene partially intercalated with Dy. The results show that nucleation is preferred on the intercalated than on the pristine areas. Difference in doping between the two areas generates an electric field that transforms random walk to directional diffusion and accounts for the guided nucleation[4]. This can be a general method to control patterning of metallic films on graphene.

In collaboration with M. Hupalo, P. A. Thiel, S. Chen, M T Hershberger, D.McDougall, C.Z.Wang.

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History and Future of Surface Quasicrystallography

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During the last decade, the fields of interface-driven 2D materials have gained tremendous attention, often due to their promising new structural or advantageous transport properties. One of these are the interface-driven 2D oxide quasicrystals (OQCs) which exhibit perfect, long-range twelve-fold rotational symmetry [1]. Such symmetry is forbidden for periodic structures. However, it can form in systems that are describable by 2D tiling patterns, which follow self-similarity supporting inflation rules.



Fig1: (left) SPA-LEED pattern of the dodecagonal quasicrystal derived from BaTiO₃ on Pt(111). Electron energy 140 eV). (right) Corresponding self-similar real-space structure of the dodecagonal Niizeki-Gähler tiling, where each vertex is decorated with a titanium atom.

For the class of perovskite oxides, we show that ultrathin films restructure into 2D quasicrystals on top of a threefold metallic substrate: Films of BaTiO₃ as well as SrTiO₃ form stable and long-range ordered dodecagonal quasicrystals on Pt(111) that are characterized by a brilliant 12-fold diffraction patterns [1,2,3]. Scanning tunneling microscopy (STM) allows to resolve the aperiodic structure of surface atoms that form a complex tiling pattern based on triangular, quadratic, and rhombic elements which is self-similar on length scales of $(2+\sqrt{3})^n$ times 0.68 nm. We show that the surface structures can be understood as a 2D cut from a 4D periodic hyperhexagonal structure. The concept and the details of the interface-driven structures will be discussed for both systems in the context of phason strain [4,5].

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Poster session of Research Unit 1700

(Monday 19:15)

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Optical Characterization and Electronic Tuning of Atomic and Molecular Chains on Si(hhl)-Au Surfaces

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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]. Moreoever, they constitute a natural template for self-assembled controllable growth of 1D chains and 2D arrays of organic molecules [3].

One technique that offers precise microscopic insight into such phenomena is reflectance anisotropy spectroscopy (RAS), which is particularly sensitive to the intrinsically anisotropic nature of surface structural motifs (Au chains, spin chains, steps), as demonstrated in previous joint theoretical-experimental studies on Si(557)-Au [4] and Si(111)Au [5].

Here I will demonstrate how first principles simulations of RAS experiments carried out within the FOR1700 network allow to characterize the structural and electronic properties of a variety of Si(hhl)-Au systems, including Si(553)-Au [6] and Si(775)-Au [7]. The electronic properties (metallicity, spin chain dampening) can further be controlled by external doping by hydrogen [6,8] and/or small organic molecules [9]. The role of the organic functional group in molecular adsorption in determining the site specificity and surface metallicity is also examined [9,10].



Left: RAS applied to Si(557)-Au. Right: Modelling dithiol adsorption on Si(553)-Au

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Formation and Interactions of Spin Chains on Stepped Silicon Surfaces

P2

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Adsorption of gold atoms on various stepped Si(hhk) substrates yields ordered atomic wire arrays, where all members of the Si(hhk)-Au family exhibit a Si honeycomb nanoribbon at the step edges [1]. The silicon atoms at the exposed edge can, under certain circumstances, be spin-polarized and charge-ordered along the edge. We have examined the formation or suppression of these so-called "spin chains". Our approach is to exploit the tunability offered by the Si(hhk)-Au family, which exhibits not only varied terrace widths but also different bonding networks, see Fig. 1.

Based on scanning tunneling microscopy (STM) and density-functional theory we reveal why spin chains form on particular Si(hhk) surfaces but not on others. Unintentional defects and controlled dopants can create or suppress local magnetic moments at Si(hhk)-Au step edges [2]. For the specific case of Si(553)-Au, the terrace is decorated by an Au double strand and features a Si spin chain with \times 3 periodicity [3]. We identify a frustrated spin interaction between adjacent spin chains which may result in the suppression of magnetic order [4]. Furthermore, we observe an interaction between the Au chains and the adjacent Si chains. In the STM data this coupling manifests itself in a modulation of the charge density at Si step edges. The spin sites feature a long-range (\times 6) pattern which lifts the inversion symmetry. Hence, spin chain exists in two different variants with opposite directionality, thereby establishing parity breaking [5]. We also succeeded in producing a novel family of Au-induced chain systems hosted on Ge(hhk) substrates, such as Ge(553), Ge(557), and Ge(335) [6].

Fig. 1 Schematic illustration of the spin chain formation in Si(hhk)-Au systems



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

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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] to well ordered two- and three-dimensional Tb silicide layers on Si(111) [3]. The metallic Tb disilicide 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. Its electronic structure near the Fermi level is characterized by sharp bands forming a hole pocket at $\overline{\Gamma}$ and strongly anisotropic electron pockets at the \overline{M} points. For monolayer depositions on Si(*hhk*) surfaces, which are 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 [Fig. 1(a)] while only irregular stripes are formed for h > k. Nevertheless, the characteristic two-dimensional electronic structure of the disilicide monolayer is observed with ARPES on all vicinal surfaces [Fig. 1(b)]. 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 for nanowire samples by an analysis of the electron pockets at the \overline{M} points.

Furthermore, electronically purely one-dimensional bands emerge for low Tb coverage on Si(335) [Fig. 1(b)]. Tb silicide structures possibly corresponding to these bands are discussed. This work was funded by the DFG, FOR1700, project E2.





Fig. 1: (a) STM image of Tb silicide nanowires on Si(335). (b) Fermi surface of a nanowire preparation on Si(335).

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A new atomic structure model for rare earth silicide nanowires on Si(001)

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Trivalent rare earth silicide nanowires are known to form by self-organization on Si(001) [1]. The formation of the nanowires was explained by assuming that they consist of hexagonal rare earth disilicides with a nearly perfect lattice match to Si(001) along their *a*-axes and a large lattice mismatch along their *c*-axes [2]. Thus, these hexagonal rare earth disilicides are expected to grow highly anisotropic on Si(001) with a long extension along *a* and a very small one along *c*, agreeing very well with the observation of nanowires and leading to the wide acceptance of this structure model [3,4]. However, this explanation of the nanowire growth is based on the lattice parameters of the bulk phases of the rare earth disilicides, which show a rather large amount of Si vacancies (about 16%). Such vacancies were never discussed for the nanowires [2-4], but stoichiometric disilicides are certainly characterized by different lattice parameters, so that the explanation for the nanowire growth and, consequently, the accepted structure model have to be questioned.

In this work, Tb silicide nanowires were prepared and characterized in a scanning tunneling microscopy (STM) setup and their inner structure was analyzed using high-resolution transmission microscopy (HRTEM) after further sample processing in air. For this purpose, the nanowires were passivated by amorphous Si, which protects them and does not change their inner structure [5].

The STM results [Fig. 1(a)] agree very well with previous studies [4]. Hexagonal structure motives and a height of two silicide layers are directly apparent in HRTEM images of the nanowires [Fig. 1(b,c)]. However, the *c*-axis of the hexagonal structure appears to be oriented along the nanowires in contrast to the up-to-now accepted structure model. Thus, we propose a new structure model, which is characterized by a 90° rotation of the silicide structure compared to its orientation in the previous one. The hexagonal Tb disilicide structure and its proposed orientation are confirmed using HRTEM image simulations of extended defocus series further enabling an assignment of characteristic features in HRTEM images to specific atom columns.

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



Fig. 1: (a) STM image of Tb silicide nanowires on Si(001). (b,c) HRTEM images of (b) the cross section and (c) the side view of Tb silicide nanowires. In the contrast enhanced insets, Tb columns are marked by yellow dots.

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From 0D to 3D: Tb induced nanostructures on Si(111)

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Like other trivalent rare earth metals, Tb forms very interesting silicide nanostructures on Si(111), ranging from zero-dimensional (0D) magic clusters to three-dimensional (3D) bulk silicides [1–4]. 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).

For very low coverages and moderate growth temperatures, 0D magic clusters form in two types, offcenter and centered Tb silicide clusters. Thereby, the latter show a bistable switching between two mirror-symmetric configurations upon tip interaction [Fig 1 (a)].

The quasi-1D 5×2 submonolayer structure [Fig. 1 (b)] consists of alternating Si chains and rows of Tb atoms in between. DFT calculations unveil a semiconducting behavior with strong electronic anisotropy. Another quasi-1D structure is formed by striped domains of the $2\sqrt{3}\times\sqrt{3}$ multilayer.

In contrast, the submonolayer $2\sqrt{3} \times 2\sqrt{3}$ superstructure and the TbSi₂ monolayer grow in a twodimensional manner, while the $\sqrt{3} \times \sqrt{3}$ multilayer forms a 3D bulk silicide structure.

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Fig1: (a) Magic clusters on Si(111)7×7. (b) The quasi-1D 5×2 submonolayer structure. (c) The 2D 1×1 monolayer and $2\sqrt{3}\times2\sqrt{3}$ submonolayer structures. (d) The $\sqrt{3}\times\sqrt{3}$ multilayer.

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Bundles of rare earth nanowires on Si(001) studied by scanning tunneling microscopy and high resolution low energy electron diffraction

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Silicides of trivalent rare earth (RE) elements form nanowires (NW) on Si(001) surfaces caused by strain effects due to the different crystal structures of Si substrate and silide [1]. After initial growth of 2D wetting layers with (2x4) and (2x7) superstructure, single NWs are formed with few-nanometer width and several 100nm length. It is assumed that the NWs have cage-like structure with RE embedded into a Si matrix. During later stages of growth form domains of bundles of NWs well aligned to each other (cf. Fig.1(a)). The number of NWs per bundle, however, shows some broad distribution.

Since the structure of the NWs is not correlated, streaks emerge in diffraction pattern. The streaks, however, show some substructure after formation of NW bundles. This substructure has been analyzed based on the binary surface technique to obtain detailed information on the width distribution of single NWs and bundles of NWs as well as the distribution of bundle distances [2]. We compare our analysis of diffraction pattern due to RE silicide NWs recorded by high resolution low energy electron diffraction with spot profile analysis (SPA-LEED, cf. Fig. 1(b)) with results obtained by scanning tunneling microscopy (STM, cf. Fig. 1(a)) [3,4].



Fig1: (a) STM micrograph showing NW bundles obtained after deposition of 2.2ML Tb on Si(001) at room temperature and annealing at 500°C. (from [4]) (b) Intensity distribution within diffraction streak (cf. inset for 2D diffraction pattern), both from [1]). Red – experimental data. Other colors – calculated intensities for various models with best fit for model shown in blue.

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Identification of vibrational modes at specific structural motifs on nominal and vicinal Si(111)-Au

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Raman spectroscopy is an extremely sensitive tool for analyzing vibrational modes of ordered (sub)monolayers of metal adatoms on semiconductor surfaces, which are typical systems for electron correlation effects. We report on the *in situ* UHV Raman analysis of self-organized Au submonolayers on nominal Si(111) surfaces, as well as on vicinal Si(553), Si(775), and Si(557). For the two-dimensional Au-($\sqrt{3} \times \sqrt{3}$) and the one-dimensional Au-(5×2) reconstructions, several specific Raman peaks in the spectral range below 200 cm⁻¹ are assigned to Au-dominated vibrational modes, while the vibrational modes around 400 cm⁻¹ were found to be associated with the Si step-edges.

Suppression of step edge fluctuations in Si(553)-Au by hydrogenation: evidence of order-disorder phase transition

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Investigations of the coupling between surface vibrational modes and the electronic properties by vibrational spectroscopy is a promising approach to understand the dynamical properties of surface stabilized atomic nanostructures. The phase transition of the Si(553)-Au surface is investigated with Raman spectroscopy and vibrational modes related to the step edges are identified. On cooling the surface below 70K, one of these modes disappears indicating a structural phase transition at the step edge. We propose a quantitative and reversible method for tuning the charge localization of Austabilized stepped Si surfaces by site-specific hydrogenation for the investigation of the phase transition mechanism. Hydrogen step-edge adsorption, having only low impact on its vibrational properties, drives excess charge into the conducting metal chain "reservoir" and renders it insulating, while surplus H recovers metallic behavior. Vibrational spectra at room temperature of the clean and hydrogenized surface exhibit the same step edge related vibrational features. At low temperature, in contrast, the phase transition in vibrational spectra observed for the clean surface is not evident for the hydrogenized surface. We discuss the possible role of the dynamic step edge fluctuations and their interplay with the electronic structure in the Si(553)-Au phase transition.

Plasmons on the Si(553)-Au surface: tuning by chemisorption

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Low-dimensional plasmons as collective excitations of charge-density oscillations contain direct information about electronic band structure, structural arrangements as well as of interactions with the embedding environment [1]. Here we report on detailed studies of plasmonic excitations and of their modifications by chemisorption on Si(553)-Au surface, using highly angular and momentum resolved EELS in combination with DFT calculations. Atomic hydrogen was found to adsorb at Si atoms, and acts as a simple (lateral) charge donor to the Au-induced chains. However, band filling turned out to be coupled with Au dimerization and band gap opening in the unoccupied part of the band structure. The theoretical predictions were fully consistent with the observations and allow a quantitative correspondence between band structure and plasmon dispersion [2].

Oxidization of the same surface, on the other hand, has an even smaller effect on metallicity and plasmon dispersion. Only extensive exposure (200 L) reduces the plasmon dispersion by only 10% [3]. Thus metallicity in both cases is only slighly affected. However, the random adsorption introduces scattering centers leading to enhances back-reflection of plasmons and the formation of standing waves, as seen in the $k\rightarrow 0$ limit.



Fig1: Plasmon dispersion obtained from the clean Si(553)-Au (black circles), after hydrogenation (left) [2] and oxidization (right) [3]. The inset in the right figure shows the evolution of Plasmon frequency as a function of oxygen exposure.

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Electronic transport in quasi-1D atomic wires

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Atomic wires on surfaces are prototype 1D systems for studying fundamental aspects, e.g. charge density waves (CDW) or dimensional crossover from a Fermi to a Luttinger liquid behavior. Among others, Au-induced wire structures on Si(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]. However, up to now the phase transition of this system is not completely understood. 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 ×2 and ×3 reconstructions at low temperature, which are associated with ordering along the Au- and Si-step edge atoms, respectively. While the ×2 periodicity persists upon annealing, the ×3 periodicity of the Si-honeycomb chain structures undergoes a structural transition at $T_{\rm C} = 100$ K. The transport experiments done at various temperatures were performed with a squared probe geometry, thus being sensitive to the crystallographic directions [2]. Upon cooling, the resistance increases at 100 K across the wires (R_{\perp}) sharply by 2-3 and along the wires (R_{\parallel}) by one order of magnitude. Both branches show saturation for T < 50 K. Since angle resolved photoemission spectroscopy revealed that metallic surface bands emerge only along the direction of wires we conclude that any R₁ behavior is related to space charge layer effects. 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]. Instead, at 65 K there is a pronounced increase of the surface state conductivity along the wires. Supported by a very recent calculation [5] which indicates a spin-liquid state is competing with a diamagnetic, i.e. spin-paired structure at low temperatures, we attribute the measured behavior to an activated charge transfer between the localized Si dangling bond states and the proximate Au-bands.

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P11 Investigation of symmetry breaking in the unoccupied electronic structure in 4/3- ML Pb/Si(111) by femtosecond time- and angle-resolved 2PPE

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Strong correlations exist between the electronic properties and structural geometry of low dimensional systems. Pb nanowires grown on vicinal surfaces have been shown to exhibit strong asymmetry in the carrier relaxation time for step up and step down directions [1]. A related problem appears for threefold symmetry of 4/3 ML Pb/Si(111)-($\sqrt{3} \times \sqrt{3}$) and we report here on the unoccupied electronic structure along [112] and [112] directions investigated by femtosecond time- and angle-resolved two photon photoemission (2PPE).

Three distinct unoccupied electronic features dispersing along $k_x \parallel [\overline{11}2]$ were identified with energies 3.65, 3.5, and 3.3 eV above the Fermi level E_F. The unoccupied nature of the identified bands were confirmed by the temporal evolution of their population dynamics curves. In angle-resolved measurements, the observed electronic states show, for opposite electron momenta $k_x > 0$ and $k_x < 0$, an asymmetric intensity distribution $I(k_x)$. An apparent symmetry break in the electronic dispersion was also observed across normal photoemission ($k_x=0$). The polarization-dependent angle-resolved measurements revealed an opposite orbital character at the opposite momenta. While other studies [2,3] discussing the symmetry breaking in angle-resolved photoemission considered a single underlying phenomenon, our analysis revealed that multiple mechanism can play a role in causing the symmetry break in the electronic band structure of our Pb/Si(111) system. These symmetry breaking phenomena might be categorized under (i) the experimental geometry or (ii) the material dependent effects. We identified a major role played by the off-normal p polarized light incidence and the asymmetry of real space structure of Si substrate along k_x direction. The asymmetry induced by the Si substrate is considered to be enhanced at its surface by Pb adsorption potentially through strong spin-orbit coupling. Also, the phenomena of final state effects in transitional matrix element has a generic importance in causing the asymmetry in photoemission intensity. However, the degree of influence of the last two discussed factors is not entirely clear and theoretical calculations are underway.

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Ultrafast Structural Phase Transition of In/Si(111) Nanowires: Exited State Band Mapping by Time- and Angle-resolved Photoemission Spectroscopy

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Quasi-one dimensional (1D) metal wires on semiconducting substrates, of which In/Si(111) is one of the most interesting and intensively studied systems, promise not only novel 1D physics, but also control over electronic properties and dimensionality. In/Si(111) undergoes a structural phase transition from a (4x1) to an (8x2) unit cell at around 120 K, concomitant with a metal-to-insulator transition. A combined DFT and Raman study [1] suggest a Peierls-like scenario, whereby a combination of shear and rotary distortions leads to the opening of band gaps and spectral shifts at specific points in the band structure. Furthermore, recent work using time-resolved electron diffraction (trRHEED) demonstrated that the photoinduced phase transition (PIPT) occurs ultrafast (<1ps) and proposed a mechanistic scenario based on *ab initio* molecular dynamics (MD) simulations [2].

Here, we utilize time- and angle-resolved photoemission (trARPES) with femtosecond extreme ultraviolet laser pulses at 500 kHz to obtain direct access to the transient electronic structure during the ultrafast PIPT from the 8x2 to the 4x1 phase [3]. Starting from the 8x2 phase we follow the gradual evolution of the electronic structure into the 4x1 phase on a femtosecond time scale. Most remarkably, the insulator-to-metal transition associated with the gap closing at the 8x2 Brillouin zone boundary occurs within 200 fs, while states at the zone center shift from above to below the Fermi level within 500 fs. Both processes occur faster than the overall structural transition into the 4x1 phase, which is completed after 700 fs. The distinct timescales of the insulator-to-metal and structural transitions clearly differ from expectations for a "standard" Peierls-like scenario for quasi 1D systems. Comparison with *ab initio* MD simulations reveals the crucial role played by localized photo-holes and opens up the possibility of addressing real space electronic distributions and bond breaking and formation dynamics on ultrashort time scales with trARPES.

Furthermore, we employ trARPES for excited state band mapping to characterize the normally unoccupied electronic structure in both structural phases of In/Si(111) and compare the extracted band positions with DFT band structure calculations. While good overall agreement is found between theory and experiment, deviations in specific momentum regions may indicate the importance of excitonic effects not accounted for at the level of the LDA or GW approximations [4].

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Indirect Chiral Magnetic Exchange through Dzyaloshinskii-Moriya–Enhanced RKKY Interactions in Transition Metal Oxide Chains on fcc(001) Surfaces

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Localized electron spins can couple magnetically via the indirect Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction even if their wave functions lack any substantial direct overlap. Theory predicts that spin-orbit scattering leads to a Dzyaloshinskii-Moriya type enhancement of the RKKY interaction [1,2], or DME-RKKY in short, giving rise to chiral exchange terms. However, experimental evidence of DME-RKKY is sparse and essentially limited to non-collinear spin structures observed in surface-deposited clusters. Here we present a combined spin-polarized scanning tunneling microscopy, angle-resolved photoemission spectroscopy, and density functional theory (DFT) study of MnO₂ chains on Ir(100). Whereas we find antiferromagnetic Mn–Mn coupling along the chain (as predicted in Ref. [7]), the inter-chain coupling across the non-magnetic Ir substrate turns out to be chiral with a 120° rotation between adjacent MnO₂ chains. DFT calculations reveal that the DM interaction results in spin spirals with a periodicity in agreement with experiment. Our findings confirm that DME-RKKY results in indirect chiral magnetic exchange, potentially giving rise to exotic phenomena, such as chiral spin-liquid states in spin ice systems or the emergence of new quasiparticles due to the trapping of single electrons in self-induced skyrmion spin textures.



Fig1: a, Large scale STM image of MnO₂ on Ir(001). Islands of monolayer height can be recognized. The entire surface including the islands are covered by chains along the [110] directions. B, Higher resolution STM image of the MnO₂ chains.

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Temperature-dependent order-disorder transition 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 metallic chains with a twofold periodicity along the terraces of the vicinal Si surface. The step edge atoms of the Si terraces are characterized by a threefold periodicity, due to the presence of unoccupied dangling bonds [1,2]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in LEED as function of temperature between 60 K and 190 K. The correlation length of Si step edge atoms along and perpendicular to the steps abruptly decreases upon heating above a temperature of $T \approx 100$ K, respectively. These findings are explained within a scenario of an order-disorder transition, where the thermal creation of solitons destroy the long-range ordering. Additionally, time-resolved ultra-fast RHEED experiments show the streak-like intensity, indicative for the twofold periodicity of the Au atoms, to decrease upon intense fs-optical excitation. This indicates transient weakening of the dimerization within the Au double-strand.

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Au atomic wires on Si(*hhk*) substrates: Recent advances from experiment and theory

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The investigation of substrate-supported quasi-1D atomic wires flourished in the last decade, owing to recent advances in experimental techniques for surface analysis, and fueled by the growing demand for outstanding materials. While many 1D properties are not spoiled by structural embedding, the coupling to the environment allows modifying physical properties, e.g., the wire metallicity. In this respect, Au wires grown on vicinal Si(111) surfaces are an ideal playground, as the miscut controls the wire width (single or double atomic rows) and the interwire distance. In this contribution, we report on theoretical and experimental studies recently performed to explore the coupling of Au wires on Si(*hhk*) surfaces with the environment. Adsorption of H and O is found to affect differently single and double Au wires [1]. The coupling of the wires to higher dimensions through the substrate results in the breakdown of the nearly-free electron gas model [2]. Thus, the wires are more appropriately described as extremely anisotropic 2D objects than as purely 1D.



Fig1: Schematic representation of the electronic band structure of the Si(553)-Au systems. (a) As measured by ARPES. The electronic states are labeled as S_{1,2} (light blue) and S₃ (blue). The Rashba split state S_{1,2} is represented by a dashed line. The DFT-PBE band structure calculated for the HCW system is shown both in the extended (b) and conventional (c) Brillouin zone representation. For the sake of clearness, only bands with strong Au character and the Si step edge state S₄ (dark blue), are shown. Surface projected bulk Si bands are in grey. The DFT-PBE band structure calculated for the LCW system is shown in (d) in a smaller energy window about the Fermi energy. The Γ -Y' direction in the HCW system and the Γ -Y'' direction in the LCW system are roughly parallel to the Au chains.

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Spin pairing versus spin chains at Si(hhk)-Au surfaces

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Surfaces involving single spin states are promising candidates for the realization of spin-based computation and storage. Both the Si(553)-Au and Si(557)-Au surface have been discussed to exhibit such unpaired spins for several years [1]. Density-functional theory is used to probe the spin structure of these surfaces. For Si(553)-Au a diamagnetic sp2 + p rehybridized structure, where the dangling bonds are either filled with two spin-paired electrons or are empty, is more favorable and in better agreement with experiment than the generally accepted spin-chain model. In contrast, the spin chains on Si(557)-Au seem rather stable against rehybridization. We discuss the mechanisms for this diverging behavior and predict methods to tailor the existence of single spin states on these surfaces. [2]



Fig1: Structure models of Si(553)-Au: Model proposed by Krawiec (K) [3], spin-chain (SC) structure due to Erwin and Himpsel [1] and rehybridized (R) surface [2] on the left together with the charge transfer from the SC to the R model and the mechanisms for parity breaking on the right.

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Novel electronic junctions in an atomic wire array: interfaces between metallic and charge density wave ordered electronic phases

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The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional electronic systems. It features a reversible, temperature-induced metal insulator transition into a charge density wave (CDW) ordered ground state with (8x2) translational symmetry. Close to the phase transition temperature, both phases can coexist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Combining scanning tunneling microscopy/spectroscopy (STM/STS) and ab initio molecular dynamics calculations, we explore the microscopic structure of interfaces between distinct electronic phases at the atomic scale. Specific defects allow to modify and control the structure of these electronic interfaces. We explain the atomistic mechanism behind the junction formation and its tunability from first principles. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

Embedded one-dimensional electronic systems

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We investigate atomic wires deposited on substrates theoretically using effective lattice models for the low-energy degrees of freedom. Our main goals are to determine under which conditions quasione-dimensional physics can be found in these materials and to identify its experimental signature.

We propose lattice models for a correlated atomic wires deposited on semiconducting substrates and show that they can be approximated by narrow ladder models that can be investigated with wellestablished methods for one-dimensional correlated systems, such as the density-matrix renormalization group [1]. We first apply this approach to the case of a correlated wire with a Hubbard-type electron- electron repulsion [2]. The ground-state and spectral properties are investigated numerically using the density-matrix renormalization group method and quantum Monte Carlo simulations. This confirms the validity of the effective ladder models for correlated atomic wires on substrates and the stability of paramagnetic Mott insulators in atomic wires.

Then we investigate the occurrence of charge density waves (CDW) and Tomonaga-Luttinger liquids (TLL) in an interacting spinless fermion wire coupled to a three-dimensional substrate using effective ladder models [3]. Our study confirms that quasi-one-dimensional TLL conductors or CDW insulators could occur in the low-energy properties of atomic wires. It also reveals that the coupling between wire and substrate stabilizes the TLL phase around the wire.

Our work also shows that the thermodynamics of one-dimensional models for atomic wires must be studied in the grand-canonical ensemble as the substrate acts as an electron reservoir for the wires. We extend the (canonical) Peierls theory for a one-dimensional metal coupled to lattice distortions to the grand-canonical case. In this grand-canonical Peierls theory both the uniform and broken-symmetry phases can become metastable and first-order Peierls transitions can occur. Starting from a Su-Schrieffer-Heeger-like model inferred from first-principles simulations, we show that the metal-insulator transition in In/Si(111) is a first-order grand-canonical Peierls transition [4]. This model explains naturally the existence of a metastable metallic phase over a wide temperature range below the critical temperature.

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