HL 71: Poster Session: Graphene / Topological Insulators / Interfaces and Surfaces

Time: Wednesday 16:00–19:00 Location: Poster D

HL 71.1 Wed 16:00 Poster D

Nanomachining of mono- and bilayer graphene with the atomic force microscope — •Johannes Rode, Hennrik Schmidt, Dmitri Smirnov, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

We investigate the effects of mechanical manipulation on mono- and bilayer graphene via atomic force microscope (AFM). Graphene flakes are obtained by micromechanical cleavage of natural graphite and are placed on a silicon substrate with a top layer of silicon dioxide. Mono- and bilayers are spotted and identified, using the optical microscope. Detailed height profiles can then be obtained by AFM, which also serves as a tool to mechanically manipulate the graphene by controlled tip movements at higher contact forces. This manipulation is performed in two ways: The effects of scratching lines into graphene with a diamond coated AFM-tip are investigated for different parameters. Furthermore we show AFM-induced folding of mono- and bilayer graphene on a μm-scale. These twisted bilayers (in case of folded monolayers) form decoupled systems which hold interesting electronic properties like a screening effect and reduced Fermi velocities.

HL 71.2 Wed 16:00 Poster D

Magnetism of Dirac Fermions — •Stephan Albert, Stefanos Chalkidis, Amadeus Mlynarski, Marc Wilde, and Dirk Grundler — James-Franck-Straße 1, 85747 Garching, Deutschland

The two-dimensional electron system of graphene exhibits a quasirelativistic dispersion relation with high mobility. Torsional cantilever magnetometry might be powerful to investigate the intriguing electronic properties via the magnetization. The ground state density of states can be mapped out which allows insight into electron-electron interaction, energy gaps and the predicted divergence of the magnetic susceptibility for vanishing magnetic field at the neutrality point. We introduce our measurement technique, and our experimental setup adapted for graphene. We report on the development of tailor-made microcantilevers by etching of SOI wafers and on sample preparation as well as the electronic characterization of exfoliated graphene prior to the magnetization measurements. Financial support by the DFG via project no. WI3320/1-1 in the priority programme "Graphene" as well as experimental support by the Nanosystems Initiative Munich is gratefully acknowledged.

HL 71.3 Wed 16:00 Poster D

Influence of structural properties on ballistic transport in nanoscale epitaxial graphene cross junctions — •Epaminondas Karaissaridis[1], Sonja Weingart[1], Claudia Bock[1], Ulrich Kunze[1], Florian Speck[2], and Thomas Seyller[2] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

We have investigated the influence of important material and device properties on ballistic transport in conventionally grown [1] and additionally hydrogen intercalated [2] epitaxial graphene cross junctions. Our studies comprise a) magneto-transport in 2D Hall bars, b) temperature- and magnetic-field-dependent bend resistance of unaligned and step edge-aligned 1D orthogonal cross junctions and c) the influence of the cross junctions' lead width on ballistic transport. We found that ballistic transport is highly sensitive to scattering at the silicon carbide step edges [3]. A suppression of ballistic transport is also observed when the lead width of the cross junctions is reduced from 50 to 30 nm. Furthermore, in a 50 nm wide 1D device prepared on quasi-freestanding graphene we observe a gradual transition from the ballistic to the diffusive transport regime when temperature is increased from 4.2 K to 30 K, although the 2D devices show a temperature-independent mean free path. Both results demonstrate that the influence of different scattering mechanisms must be studied in detail.

[1] K.V. Emtsev, *et al.*, Nature Mater. **8**, 203 (2009).
[2] F. Speck, *et al.*, Mat. Sci. Forum **645-648**, 629 (2010).
[3] S. Weingart, *et al.*, Appl. Phys. Lett. **95**, 262101 (2009).

HL 71.4 Wed 16:00 Poster D

Landau level splitting in monolayer and bilayer graphene superlattices — •George Pal, Walter Apel, and Ludwig Schweitzer — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

The application of periodic potentials to graphene tailors its electronic and transport properties in a unique way, leading to novel features and interesting physics. We employ a lattice model to investigate the Landau level spectrum of graphene in perpendicular magnetic fields and an additional one-dimensional superlattice made of square potential barriers. When the potential barriers are oriented along the arm-chair direction of graphene, we find for strong magnetic fields that the zeroth Landau level of both monolayer and bilayer graphene splits into two well separated sublevels. This splitting occurs only when the superlattice barrier width is smaller than the magnetic length. In this situation, which persists even in the presence of disorder, a plateau with zero Hall conductivity is supposed to be observed around the Dirac point. The splitting occurs also in the presence of truly two-dimensional (chess-board type) superlattices, and it remains robust even in the presence of additional on-site disorder. The superlattice induced Landau level splitting is a true lattice effect that cannot be obtained from the usual continuum Dirac-fermion model of graphene.
[1] G. Pal, W. Apel, and L. Schweitzer, submitted (2011)

HL 71.5 Wed 16:00 Poster D

Non-local Andreev reflection as a probe of spin entanglement in graphene nanostructures — •Hans Hettmansperger[1], Patrik Recher[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

The controlled production and detection of spin-entangled electronic states without the use of ferromagnetic reservoirs is a major challenge in solid state physics. Non-local Cooper pair injection from ordinary superconductors into graphene nanostructures can be used to generate spin entanglement. The advantage of graphene is twofold: (i) spin is long-lived in graphene because it only weakly couples to the environment; (ii) graphene nanoribbons have specific properties that allow for a spin detection in the absence of ferromagnetic reservoirs.

In our numerical analysis, we solve the Bogoliubov-de Gennes equation for the tight binding model of graphene by applying the recursive Green's functions method for phase-coherent transport to multi-terminal devices. We study the average current and the current noise within and between different electron reservoirs and identify ideal situations to generate and detect spin entanglement. To do so, we employ graphene-specific physics such as valley filtering and magnetic ordering due to electron-electron interactions in zigzag nanoribbons.

HL 71.6 Wed 16:00 Poster D

Resonant scattering in graphene: adsorbate fingerprints from ab initio calculations — •Karri Saloriutta[1], Martti J. Puska[1], and Antti-Pekka Jauho[2] — [1]Department of Applied Physics, Aalto University School of Science, Finland — [2]Department of Micro- and Nanotechnology, DTU Nanotech, Technical University of Denmark, Denmark

We have recently shown that by using a scaling approach for randomly distributed defects reliable estimates for transmission properties can be calculated based on even single defect calculations. This is done by defining a scattering cross-section, a quantity that only depends on energy and defect type. Estimates of transmission and all the related transport properties, such as localization lengths and mean free paths, can then be calculated for a macroscopic system with an arbitrary defect density.

We now extend our analysis to the case of adsorbates on graphene by studying the experimentally important epoxide and hydroxyl groups. We show that a qualitative understanding of resonant scattering can be gained even from a single bulk graphene calculation, which thus provides an useful transmission "fingerprint" for each adsorbate. For graphene nanoribbons on the other hand the scattering cross section needs to be calculated from an ensemble containing all the relevant adsorption sites across the whole ribbon. The transmission in ribbons is also strongly affected by the van Hove singularities at band edges making the scattering cross section specific to a particular ribbon width.

HL 71.7 Wed 16:00 Poster D

Defect controlled conductivity of graphene with vacancies

and N impurities — •Karel Carva[1], Biplab Sanyal[2], Jonas Fransson[2], and Olle Eriksson[2] — [1]Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

The possibility to influence the electronic structure of graphene and hence control its conductivity by adsorption or doping with adatoms is crucial in view of electronics applications. We study electronic structure and transport properties of single and bilayer graphene with vacancy defects, as well as N doped graphene. The theory is based on first principles DFT calculations employing coherent potential approximation (CPA) to describe disorder. We show that increasing the defect concentration increases drastically the conductivity in the limit of zero applied gate voltage [1], by establishing mid-gap states and carriers in originally carrier-free graphene, a fact which is in agreement with recent observations [2]. We calculate the amount of defects needed for a transition from a non-conducting to a conducting regime (i.e. a metal-insulator transition) and establish the threshold of the defect concentration where the increase of impurity scattering dominates over the increase of carrier induced conductivity [1].

[1] K. Carva, B. Sanyal, J. Fransson, O. Eriksson, Phys. Rev. B 81 (2010) 245405.

[2] S. H. M. Jafri et al., J. Phys. D: Applied Physics 43 (2010) 045404.

HL 71.8 Wed 16:00 Poster D

Superlattice Effects on Transport in Graphene and Graphene Nanoribbons — •Fedor Tkatschenko, Jan Bundesmann, Viktor Krückl, Dmitry Ryndyk, and Klaus Richter — Universität Regensburg Germany

Motivated by interesting superlattice effects on bulk graphene such as the emergence of new Dirac points and an anisotropic velocity renormalization[1], we numerically investigated the effects of a one dimensional superlattice potential on the electronic properties of graphene nanoribbons (GNR). We found that the formation of the miniband structure depends on the direction of the ribbon axis. The arising miniband structures of armchair GNRs exhibit striking differences, depending on whether the ribbon is metallic or semiconducting. In case of zigzag GNR the miniband structure forms only for ribbons where the width has an even number of chains. We also investigated the current voltage characteristic through modulated GNR which shows a negative differential conductance and an oscillatory behavior due to Bloch-oscillations in presence of Zener tunneling[2].

[1] M. Barbier, F.M. Peeters, P. Vasilopoulus and J.M. Pereira, Phys. Rev. B **77**, 115446 (2008),

[2] Viktor Krückl and Klaus Richter, arXiv:1109.5541v1

HL 71.9 Wed 16:00 Poster D

Modulating Charge Carrier Concentration using Patterned Top Gates in Graphene Structures — •Franz-Xaver Schrettenbrunner, Dominik Koch, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

We report on the fabrication and the measurements of graphene single layers with structured top gates. Starting from exfoliated graphene on SiO_2 surfaces, a thin Al_2O_3 top gate dielectric was fabricated by atomic layer deposition (ALD). Subsequently a top gate electrode consisting of an array of lateral stripes with periodicities down to 100 nm was fabricated by electron beam lithography (EBL). The interplay of both patterned top- and extended back gate allows to tune type and concentration of charge carriers as well as the modulation strength. Different configurations like n^+nn^+, npn or p^+pp^+ can be realized. For npn configuration in single layer graphene, magnetotransport measurements show an unusual linear increase and additional dips in the magnetoresistance. Furthermore, we obtain quantum Hall states corresponding to locally modulated filling factors achieved by tuning the patterned top gate.

HL 71.10 Wed 16:00 Poster D

Crystallographically Anisotropic Etching of Graphene — •Florian Oberhuber, Paula Giudici, Stefanie Heydrich, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universtität Regensburg, 93040 Regensburg, Germany

We report the crystallographically anisotropic etching of exfoliated graphene on SiO_2 substrates by a carbothermal reaction. The etching mechanism was suggested to take place between graphene and oxygen from the SiO_2 substrate and leading to graphene with zigzag edges [1]. Before exposing samples to this carbothermal reaction, they were patterned with circular antidots by electron beam lithography and reactive ion etching with oxygen plasma. In the following carbothermal etching samples were exposed to temperatures around 800°C in a flow of argon gas (purity 6.0) and the predefined holes evolved into larger hexagonal antidots. Samples were characterized by Raman spectroscopy focussing on G ($\sim$1580cm^{-1}), D ($\sim$1350cm^{-1}) and D' ($\sim$1620cm^{-1}) peaks. On the other hand we investigated electron transport on a set of samples patterned with square lattices of hexagonal holes. By analizing the weak localization peak we obtain the phase coherence length as well as lengths for intra- and intervalley scattering. The results will be compared to graphene patterned with circular holes investigated previously [2].

[1] P. Nemes-Incze et al., Nano Res. 3 (2010)

[2] J. Eroms et al., New J. Phys. 11 (2009)

HL 71.11 Wed 16:00 Poster D

Nanoscale control of the dielectric environment of graphene — Vitalij Scenev, •Nikolaj Severin, and Jürgen Rabe — Humboldt Universität Berlin zu Berlin, Institut für Physik, D-12489 Berlin

The quantitative understanding of charge transfer at interfaces and the spatial distribution of the resulting charge carriers is a critical input to electronic device design. Particularly, the performance and reliability of a graphene field effect transistor (FET) can be dominated by the graphene/substrate environment. Electrostatic force microscopy (EFM) is a versatile tool for quantitative and qualitative investigations of electronic properties of surfaces on the nanoscale, providing high spatial resolution, with no need for electrical contacts. We exfoliated graphenes onto muscovite mica under variable relative humidities. Topography images of graphenes reveal flat plateaus of three different heights, which can be attributed to molecular water layers confined between graphene and mica. EFM revealed reproducible surface potential differences between the plateaus. The variation of the surface potential may be attributed to charge transfer between graphene and the underlying substrate and the orientation of polar water molecules within the molecular layers. We show that the water monolayers can modify the interface between graphene and the substrate and may control the doping level of graphene on the nanoscale.

HL 71.12 Wed 16:00 Poster D

Transport Properties of Graphene on Atomically Flat Substrates — •Jens Mohrmann[1], Hilbert v. Löhneysen[1,2], and Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany — [2]Physikalisches Institut, KIT, Germany

Graphene is commonly described as a perfect two dimensional crystal. But although this is true with respect to the electronic properties, TEM and SPM investigations showed that the structure in real space is not perfectly flat. Instead, both suspended and SiO2 supported graphene show ripples. In case of substrate supported graphene, these ripples originate from graphene conforming to the substrate's roughness. Different mechanisms that may lead to interactions between the topographical corrugations and electronic transport properties have been proposed, and recently atomically flat hexagonal boron nitride was found to be an ideal substrate, leading to extremely high charge carrier mobilities. Yet, the influence of the ripples on electronic properties is under debate. Using a graphene transfer technique, we investigate this effect by placing graphene on hexagonal boron nitride and mica and comparing electronic transport measurements and roughness.

HL 71.13 Wed 16:00 Poster D

Contact Resistance in Graphene Field Effect Transistors — •renjun du[1], kristina hönes[1], pablo robert[1,2], fan wu[1], hilbert von löhneysen[1,2,3], and romain danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

A high-quality junction between graphene and metallic contacts is crucial in the creation of high-performance graphene field effect transistors. In an ideal metal-graphene junction, the contact resistance is determined solely by the number of conduction modes in graphene. However, measurements of contact resistance have been inconsistent, and the factors that determine the contact resistance remain unclear. In this work, we achieved conduct patterns on the exfoliated graphene

by performing e-beam lithography and evaporated palladium through ultra high vacuum (UHV) system. The contact resistance between palladium and graphene is measured at room temperature. Additionally, the dependence of extracted mobility on channel dimensions is studied.

HL 71.14 Wed 16:00 Poster D

Ultrafast phonon relaxation in graphite — •Martin Scheuch[1], Tobias Kampfrath[1], Martin Wolf[1], Konrad von Volkmann[2], Christian Frischkorn[3], and Luca Perfetti[4] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [2]APE GmbH Plauener Str. 163-165 Haus N, 13053 Berlin — [3]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [4]Laboratoire des Solides Irradiés, Ecole polytechnique, 91128 Palaiseau cedex, France

A nonequilibrium population of high energy optical phonons (SCOPs) is generated in graphite following the excitation of electron-hole pairs with an 800-nm, 10-fs pump pulse. The energy relaxation of these phonons can be probed by means of time-resolved terahertz spectroscopy of the electronic subsystem because an equilibrium between electrons and SCOPs is established immediately after excitation [1]. To avoid transport effects, measurements are taken on homogenously excited thin films. We find an increase of the hot-phonon lifetime by a factor of two when the sample temperature decreases from 300 K to 5 K. These results suggest that the energy relaxation in graphite is dominated by the anharmonic decay of hot A_1' phonons at the K point into acoustic phonons with energies of about 10 meV [2]. Our results are qualitatively valid for graphene as well [3].

[1] T. Kampfrath *et al.*, Phys. Rev. Lett. **95**, 187403 (2005).
[2] M. Scheuch *et al.*, Appl. Phys. Lett. **99**, 211908 (2011).
[3] N. Bonini *et al.*, Phys. Rev. Lett. **99**, 176802 (2007).

HL 71.15 Wed 16:00 Poster D

The detection of terahertz radiation via graphene based devices at low magnetic field — •Majdi Salman[1,2], Markus Golla[2], Yu. B. Vasilyev[3], Fathi Gouider[2], Miriam Friedemann[4], Franz. J Ahlers[4], Hennrik Schmidt[2,5], Rolf Haug[5], and Georg Nachtwei[2] — [1]NTH Nano School for Contacts in Nanosystems, Germany — [2]Institut fuer Angewandte Physik, Technische Universitaet Braunschweig, Braunschweig, Germany — [3]Ioffe Physical Technical Institute, Russian Academy of Science, St. Petersburg, Russia — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [5]Institut für Festkörperphysik, Universität Hannover, Appelstraße 2, Hannover, Germany

The influence of a magnetic field on Landau levels (LLs) in graphene-based devices is described via the magneto- optical response induced by terahertz (THz) radiation. For single-layer graphene, the resonance energies of the transitions between the LLs such as L1, L2 and L3, fit quite well to the terahertz spectral range at low magnetic fields. Also, the calculations for the terahertz photoresponse in the in presence of low magnetic field, the reported calculations for the scattering rate of LLs, recent and our primary experimental results of transmission and photoresponse measurements implying that single-layer graphene can be suitable for the detection of terahertz radiation. On the other hand, temperature dependence of full width at half maximum (FWHM) of infrared transmission measurements were utilized in our calculation to argue that the graphene based devices can be also suitable for the detection of terahertz radiation at room temperature.

HL 71.16 Wed 16:00 Poster D

Edge Functionalization of Graphene Nanoribbons — •Eric Parzinger, Max Seifert, Lucas Hess, Martin Stutzmann, and Jose Antonio Garrido — Walter schottky Institut, TU München, Germany

Due to its unconventional electronic properties, graphene is a suitable material for investigating low dimensional effects e.g. quantized conductance even at room temperature. When shrinking down the dimensions of graphene field effect transistors to the nanoscale, the sheet edges gain more and more importance and are known to have a strong influence on the device performance. It has been shown that proper functionalization of the edges and, thus, passivation of dangling bonds can greatly improve the performance of nanoscale devices. We use CVD grown graphene and electron beam lithography to produce nanoscale graphene field effect transistors, and we investigate the effect of different functionalization methods on the electronic properties of such devices.

HL 71.17 Wed 16:00 Poster D

Cell Bioelectronics using Graphene Transistors — •Liding Zhang, Lucas Hess, Max Seifert, Christoph Becker-Freyseng, Martin Stutzmann, Ian D. Sharp, and Jose A. Garrido — Walter Schottky Institut, TU München

In this work, we present results on the interaction of graphene solution-gated field effect transistors (G-SGFETs) with living cells. The biocompatibility of graphene was tested by growing different types of cells on bare graphene substrates as well as on arrays of G-SGFETs. Cardiomyocyte-like HL-1 cells, Human Embryonic Kidney (HEK) cells and pure retinal ganglion cells from postnatal rats have been cultured successfully. Using the transistors beneath, action potentials generated by the cells could be detected and resolved. By means of the patch clamp technique, additional detail on these action potentials is obtained leading to a more detailed understanding of the cell-transistor interface.

HL 71.18 Wed 16:00 Poster D

Direct growth of few-layer graphene on mica — Gunther Lippert, •Marvin Zöllner, Jarek Dabrowski, and Grzegorz Lupina — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

In many potential technological applications of graphene a transfer-free, low-temperature graphene deposition method on insulating substrates is required. We present a Van der Waals epitaxy-based approach enabling direct growth of few-layer graphene on freshly cleaved mica surfaces at temperatures below 1000°C. Graphene growth is accomplished in an ultra high vacuum molecular beam epitaxy chamber equipped with a high purity pyrolytic graphite source. According to the optical microscopy and Raman spectroscopy, the deposition of carbon onto mica surfaces results in the formation of micrometer-size islands of few-layer graphene (<10 monolayers). Analysis of the relative intensities of the characteristic 2D, G, and D Raman peaks implies a good crystalline quality of the deposited layers. The experimental insights are combined with ab-initio calculations to propose a model for graphene growth on mica surfaces.

HL 71.19 Wed 16:00 Poster D

Resist-free patterning and transport measurements on graphene layers — •Benedikt Sommer, Arkadius Ganczarczyk, Martin Geller, and Axel Lorke — Faculty of Physics and CeNIDE, Universität Duisburg-Essen

Graphene is expected to have an exceptional high charge carrier mobility even at room temperature. However, high mobility in patterned graphene layers may be hampered by the patterning process, as many processes involve a lithographic step, which requires that the graphene is covered with an organic resist. This step may compromise the transport properties of graphene permanently, as the resist can not be removed completely. A lot of effort is being invested into finding ways to pattern graphene in a mask- and resist-free manner.

In this work, we show resist-free patterning of graphene sheets using different techniques within a focused ion beam (FIB) system. Care has been taken that the active area of the graphene has not been exposed to either ion or electron beams. Furthermore, the graphene has not been exposed to organic materials or solvents after the exfoliation process. The patterned graphene layers are characterized in transport measurements from low temperatures (4 K) up to room temperature, especially to extract the mobility of the charge carriers.

HL 71.20 Wed 16:00 Poster D

Transport through structured ultra-thin Bi_2Se_3 flakes — •Regine Ockelmann[1,2], Christian Volk[1,2], Anton Maier[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]PGI, Forschungszentrum Jülich, 52425 Jülich, Germany

Topological insulators (TIs) are a new class of solid state materials with unique electronic properties showing both carriers mimicking relativistic particles and topological protection of their surface states. Theory predicts topological insulators to exhibit a rich variety of physical phenomena such as anomalous magneto-electric coupling, Majorana excitations and unusual spin-orbit interaction. Bismuth (Bi) based compounds such as Bi_2Se_3 have been shown to be interesting topological insulators with a single Dirac cone surface state and strong spin-orbit interaction.

Here, we present low-temperature transport measurements on structured ultra-thin $3nm$-$20nm$ Bi_2Se_3 flakes, such as Hall bars. The ultra-thin flakes have been prepared by exfoliation of bulk Bi_2Se_3 and are

placed on SiO_2 on highly doped Si substrates. The final devices are structured with electron beam lithography followed by ion beam etching and contacted by Ti/Au electrodes. Low temperature $\sim 1,5K$ transport, i.e. conductance measurements have been carried out by driving back gate voltages from $-70V$ to $70V$ and by varying magnetic fields up to $9T$. We observe an ambipolar electric field effect and deduce a carrier mobility of around $\sim 3000cm^2/(Vs)$, and a carrier concentration of around $\sim 3 \cdot 10^{13}cm^{-2}$.

HL 71.21 Wed 16:00 Poster D

MBE-grown HgTe as a 2D and 3D topological insulator — •Philipp Leubner, Christopher Ames, Maximilian Kessel, Matthias Mühlbauer, Luis Maier, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — Physikalisches Institut (EP III), Universität Würzburg, D-97074 Würzburg, Germany

Since the first theoretical prediction of the quantum spin hall effect in 2005 [1], topological insulators (Tis) are receiving ongoing attention due to their unique band structure. In 2007 the first experimental evidence of a 2D TI was found in an HgTe/HgCdTe heterostructure [2].

We have grown HgTe layers of different thicknesses on CdTe substrates via molecular beam epitaxy in order to investigate the transition between 2D and 3D TIs. The effect of strain and relaxation due to lattice mismatch is crucial for the band properties of HgTe and therefore analyzed via HRXRD.

Additionally, we present transport measurements on the grown layers showing indications of 2D or 3D TI behavior depending on layer thickness.

[1] Kane et. al., Phys. Rev. Lett. 95 146802 (2005) [2] König et. al., Science 318, 766 (2007)

HL 71.22 Wed 16:00 Poster D

Kondo Tunneling between 1D Helical Liquids — •Thore Posske, Chao-Xing Liu, Jan Carl Budich, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Wuerzburg

Two non-interacting helical edge liquids are coupled via a magnetic impurity. Different chemical potentials are attached to every Fermion species to imitate a four terminal setup and drive the system out of equilibrium. In a special limit of the coupling constants, the Toulouse limit, the system is mapped to a non-interacting one using Bosonization and Refermionization. We explicitly calculate the spatially dependent Kondo screening cloud that is emerging in the edge channels. This allows us to show how the helicity can be used to gain additional information about the Kondo cloud using transport measurements.

HL 71.23 Wed 16:00 Poster D

Analysis and Improvement of the modified Becke-Johnson exchange potential — •David Koller, Fabien Tran, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, A-1060, Vienna, Austria

The modified Becke-Johnson exchange potential [1] (TB-mBJ) is the sum of an approximation to Slater's averaged exchange potential and a response contribution, with the weight of both parts determined by the parameter $c = c(\overline{\nabla\rho/\rho})$. It is a semilocal potential which leads to surprisingly good energy gaps for semiconductors and insulators. Its predictive power is better than that of hybrid-DFT calculations and similar to the much more expensive GW approach. The improvement is explained by the different spatial distribution of electrons in the valence band maximum and conduction band minimum states. For correlated TM compounds TB-mBJ works similarly to LDA+U and improves magnetic moments, band gaps and electric field gradients but (correctly) does not shift the occupied states below the O-p-band.

Although the performance of TB-mBJ is impressive, some cases would be described even better by a different choice of c. Therefore we investigated three strategies for improvement: reparametrization of the relation between c and $(\overline{\nabla\rho/\rho})$, determining c from a different quantity and using a position-dependent $c(\mathbf{r})$. The first strategy turns out to be helpful, especially when grouping the systems into categories like sp-semiconductors, wide band gap insulators or (non-)magnetic transition metal compounds.

HL 71.24 Wed 16:00 Poster D

A functional renormalization group approach for treating interactions in strongly disordered electron systems — •Christian Seiler[1,2] and Ferdinand Evers[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany

We propose an approach to treat the effects of interactions in disordered electron systems on a numerical level. The idea is to solve the non-interacting disorder problem for a given disorder realization exactly. We then use the functional renormalization group method to introduce interactions on a perturbative level. In contrast to usual applications of the fRG, we formulate it in terms of the eigenfunctions of the disordered non-interacting Hamiltonian. Disorder averaging of physical quantities is performed as the final step. The main advantage of our approach is that we are able to treat disorder exactly from a numerical point of view. We compare our method to exact diagonalization and Hartree-Fock for small systems and discuss its applicability for larger systems.

HL 71.25 Wed 16:00 Poster D

FTIR-Spectroscopy of MOCVD-Prepared Ge(100) and P-rich GaP(100) — •Claas Löbbel[1], Anja Dobrich[1], Johannes Luczak[1], Sebastian Brückner[1,2], Henning Döscher[1,2], Peter Kleinschmidt[1,3], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, D-99099 Erfurt

We have investigated hydrogen bonding in MOVPE-prepared Ge(100) surfaces as well as GaP/Si(100) surfaces using Fourier-transform infrared (FTIR) spectroscopy in an attenuated total reflection (ATR) configuration enabling sensitive measurements of the germanium-hydrogen bonds as well as phosphorus-hydrogen bonds at the surface. MOVPE preparation and in-situ reflectance anisotropy spectroscopy (RAS) measurements were correlated with UHV-based surfaces science techniques such as FTIR, scanning tunnelling microscopy (STM), and low-energy electron diffraction (LEED) by employing a contamination-free MOVPE to UHV transfer system. FTIR measurements showed Ge-H monohydrides as well as P-H semihydrides surfaces, agreeing with results from LEED. Polarization dependend Ge(100) FTIR measurements revealed, matching STM results, a (2x1)/(1x2) reconstructed surface and even allowed a quantization of the domain ratio.

HL 71.26 Wed 16:00 Poster D

Atomic surface structure of Ge(100) surfaces in vapor phase epitaxy ambient — •Sebastian Brueckner[1,2], Oliver Supplie[1], Enrique Barrigon[3], Henning Doescher[1,2], Anja Dobrich[1], Claas Loebbel[1], Johannes Luzcak[1], Peter Kleinschmidt[1,4], and Thomas Hannappel[1,2,4] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]Instituto de Energía Solar, Universidad Politécnica de Madrid, E-28040 Madrid — [4]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Vicinal Ge(100) substrates represent almost perfect templates for III-V nucleation and are therefore established as substrates for III-V triple junction solar cells grown by metal-organic vapor phase epitaxy (MOVPE). An important requirement to achieve low defect densities in the III-V epilayers is a suitable Ge(100) surface preparation prior to heteroepitaxy. We applied in situ reflectance anisotropy spectroscopy (RAS) to study the Ge(100) surface during preparation. A contamination free MOVPE to ultrahigh vacuum (UHV) transfer system allowed us to correlate the spectra to results from various surface science methods. Processing of Ge(100) in MOVPE environment under hydrogen led to a surface free of oxides and carbon, covered by monohydrides. Vicinal Ge(100) exhibits a preferential (2×1) surface reconstruction domain, i.e. D_B steps. Exposure to arsenic resulted in predominat (2×1) or (1×2) surface reconstruction domains which was controlled in situ by RAS dependent on temperature and source of As (AsH_3 or As_4).

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Surface chemical and electronic properties of In_2O_3 and In_2O_{3-x} nanoparticles for ozone detection — •Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Oliver Ambacher[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastr. 72, 79108 Freiburg, Germany

The electrical properties of indium oxide nanoparticle films can be

tuned by variation of growth temperature as well as rapid thermal annealing, UV-irradiation and ozone-induced oxidation. The high O_3 sensitivity of indium oxide thin films is strongly linked to their structural and electronic properties. Especially, the alteration of the surface electron accumulation plays an important role in the change of the film resistivity upon O_3 interaction and UV-induced regeneration. We analyse the changes of indium oxide surface properties with respect to varying crystallinity using AFM, XPS and UPS. Compared to stoichiometric In_2O_3 thin films, indium oxide nanoparticles exhibit a high oxygen deficiency and hence a high defect density at the nanoparticle surface. After growth, these defects are saturated by hydrocarbons due to the incomplete decomposition of precursors during low temperature MOCVD. The defects and the changed stoichiometry have impact on the surface band alignment. Upon ozone-induced oxidation and UV photoreduction a reversible change in band bending, surface dipole and O adsorbate density is found and will be discussed in context with electron transport characteristics and thermal properties.

HL 71.28 Wed 16:00 Poster D

Gallium Phosphide - Silicon Interface: Structure and Anisotropy Investigations — •Steinbach Gabi[1,2], Gemming Sibylle[1], Döscher Henning[3], Hannappel Thomas[3,4], and Schreiber Michael[2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, D-01314 Dresden. — [2]Institute of Physics, TUC, D-09107 Chemnitz. — [3]HZB, D-14109 Berlin. — [4]Ilmenau University of Technology, Inst. of Physics, Dep. Photovoltaics, D-98684 Ilmenau.

Gallium phosphide thin films on cheap silicon substrates are a promising III-V/IV heterostructure to be used in optoelectronic devices. As an almost lattice matched system with a band gap difference of 1.14 eV it includes applicability for multi-junction solar cells. The present study concerns discontinuities emerging at the boundaries of a GaP thin layer on a silicon substrate. The optical anisotropy of the (001) interface has been determined by an optical model applied to reflectance anisotropy spectroscopy measurements of the GaP/Si heterostructure. Density-functional calculations of the interface have been performed with both, the pseudopotential plane wave code ABINIT [1] and the all-electron augmented plane wave code Wien2K [2]. The study distinguishes between the Ga-rich and the P-rich interface termination. At the perfectly flat interface, the latter exhibits higher stability as indicated by the work of separation. More complex interface models also consider defects. The calculated density of states projected onto in-plane directions gives an indication for anisotropy. It aims at distinguishing interface termination and defects as origin of the experimentally observed reflectance anisotropy. [1] www.abinit.org [2] www.wien2k.at

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Calculation of valence band offsets from tight-binding band structures — •Daniel Mourad and Gerd Czycholl — Institut für Theoretische Physik, Universität Bremen

The anisotropic valence band offset (VBO) across an interface between two semiconductors A and B is an important material parameter, as it (among others) determines the confinement potential and so e.g. the heterostructure type (I or II) and the level structure in low-dimensional systems. Furthermore, the electronic properties of semiconductor alloys are directly influenced by the VBO. A crucial ingredient in the calculation of the VBO is the use of sufficiently accurate band structures. We present different methods of calculation for the VBO by means of a determination of the charge neutrality level in the framework of an empirical tight-binding model (ETBM).The values will be compared for different sets of material parameters and crystalline phases (zincblende and wurtzite). Furthermore, we will use them to calculate the electronic properties of A_xB_{1-x} semiconductor alloys.

HL 71.30 Wed 16:00 Poster D

The Change of Electrical Conductivity in Dependence of UV Illumination of Nano-Porous Titania (TiO_2) Combined with Infrared Spectroscopy (FTIR) — •Thomas Kriesche[1] and Thomas Bürgi[2] — [1]Phys.-Chem.-Institut, Im Neuenheimer Feld 253, 69120 Uni Heidelberg — [2]Faculté des Sciences, Séction de Chimie, Département de Chimie Physique, Quai Ernest-Ansermet 30, CH-1211 Genève 4

The properties of nano-porous TiO_2 is widely investigated by FTIR. In particular this method is used to observe photocatalytic processes on TiO_2. The spectrometer IFS66v Bruker is expanded with an electrometer (Keithley2100), which measures the electrical conductivity during IR-spectroscopy. Absorbed UV-light creates electrons and holes in the semiconductor, which recombine or can do reduction respectively oxidation of adsorbed molecules on surface. The conductivity is measured on top of a TiO_2 pill via a four point method, those is fixed in a Diffuse Reflectance IR (DRIFT) unit (PIKE EasiDiff). The well known degradation of malonic acid [1] has been studied with this setup. The recent work presents results from ATR-FTIR and DRIFT in MIR with the change of the electrical conductivity during UV illumination. [1] I.Dolamic, T.Bürgi: Photoassisted Decomposition of Malonic Acid on TiO_2 Studied by in Situ Attenuated Total Reflection Infrared Spectroscopy, J. Phys. Chem. B 2006