# HL 62: Graphene: SiC substrates and intercalation (O, jointly with HL, TT)

Time: Wednesday 16:00–19:15 Location: H17

HL 62.1 Wed 16:00 H17

**Molecular Doping of Epitaxial Graphene on SiC with flouro-fullerenes** — •Martina Wanke[1,2], Anton Tadich[3], Mark Edmonds[4], Yaou Smets[4], Chris Pakes[4], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany — [2]LS Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse 1, 91058 Erlangen — [3]Soft-X-Ray-Beamline, Australian Synchrotron, 800 Blackburn Road, Clayton, VIC 3168, Australia — [4]Scholl of Physics, La Trobe University, Physical Sciences 1, Bundoora, VIC 3086, Australia

Epitaxial graphene (EG) on SiC(0001) is intrinsically n-type doped due to charge transfer from the substrate surface [1,2]. Charge transfer doping with F4-TCNQ reduces the carrier concentration and increases the carrier mobility [2], but the stability of the molecular layer in ambient conditions is not given [2]. Molecules with a sufficiently high electron affinity are needed in order to achieve a significant reduction of the electron concentration in EG by surface transfer doping. The mechanism of surface transfer doping of diamond with $C_{60}F_{48}$ is well understood [3]. Using ARPES we investigated the surface transfer doping of EG with $C_{60}F_{48}$. A net p-type doping of EG was observed for higher coverages of the $C_{60}F_{48}$.
[1] T.Ohta et al., Science **313** (2006) 951; [2] J.Jobst et al., PRB **81** (2010) 195434; W.Chen et al., JACS **129** (2007) 10418; C. Coletti et al., PRB **81** (2010) 235401. [3] M. T. Edmonds et al., JCP 136 (2012) 124701.

HL 62.2 Wed 16:15 H17

**Transport properties of epitaxially grown graphene nanostructures** — •Jens Baringhaus, Frederik Edler, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The patterning of graphene into small stripes, the so called graphene nanoribbons, is an essential task for the development of future graphene based electronic devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. The fabrication of these well-defined structures requires the avoidance of any damaging post-processing. To overcome this obstacle we use a selective graphitization process on SiC-mesa structures, producing monolayer graphene nanoribbons of 40 nm to 100 nm in width and of several micrometers in length. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. The self-assembled graphene nanoribbbons show metallic behavior and can be clearly distinguished from the non-metallic substrate. Conductances close to $G_0 = e^2/h$ are observed for a wide temperature range from 30 K up to room temperature. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single ballistic channel. This is a strong indication for spin-polarized transport through the edge-states of the ribbons. These edge states also show up in scanning tunneling spectra. At higher temperatures the conductance increases due to the occupation of the next subband. Remarkably all investigated ribbons exhibit very large mean free paths up to 15 $\mu m$.

HL 62.3 Wed 16:30 H17

**Local investigation of transport properties and morphology of epitaxially grown 2d graphene** — •Frederik Edler, Jens Baringhaus, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Graphene has a peculiar band structure and special transport properties. The transport is strongly affected by imperfections of the graphene films, e.g atomic steps and impurities located at the interface between graphene and its support. A reliable control of these parameters is possible by epitaxial grown graphene on SiC. To characterize the epitaxial growth and correlate the structure with transport properties, the sheet resistance of graphene grown on SiC(0001) and SiC(000$\bar{1}$) have been studied via a 4-tip STM/SEM system. The SEM allows precise positioning of feedback controlled STM tips, enabling transport measurements on a nm-scale. While STM is used to characterize atomic size defect structures, step-bunches and nano-inhomogeneities can be identified in SEM. Sheet resistances were found to be independent from probe spacing indicating a 2d transport behavior but highly depending on ex-situ processing steps. Further in-situ annealing led to sheet resistances around $6 - 8$ kΩ/□. These values can be explained by diffusive transport theory [1] and correlate with the concentration of the nano-inhomogeneities. Structural defects induce a mobility gap as deduced from temperature-dependent transport measurements. The sheet resistance increased by a factor of three for elastically bend graphene layers across SiC step-bunches. [1] Adam *et al.*, PNAS, **104**, 18392 (2007)

HL 62.4 Wed 16:45 H17

**Electronic structure of epitaxial graphene on 3C-SiC(111)** — •Lydia Nemec, Volker Blum, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

We present a study of the electronic structure of the carbon-rich surface phases on 3C-SiC(111), including quasi-freestanding graphene and intercalated phases. Our approach is based on density-functional theory (DFT) including van der Waals (vdW) dispersion terms in the Tkatchenko-Scheffler approach [1]. We use semilocal DFT (PBE+vdW functional) for our first-principles structure predictions. For the oxygen intercalated bilayer graphene, we consider an oxygen-rich interface passivating the Si dangling bonds [2]. Based on the predicted geometries, hybrid functionals (HSE06 and PBE0) are used to assess the electronic structure of: (1) the partially sigma-bonded "buffer layer" phase, (2) quasi-freestanding graphene up to three monolayers, and (3) hydrogen- and oxygen intercalated graphene phases. For the different phases, we discuss the changes of the electronic structure, addressing the influence of the intercalated material on the doping of the graphene and the charge transfer from the substrate to the graphene layer. We observe that in the intercalated phases graphene is decoupled from the substrate, making intercalation a promising approach for further studies.
[1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).
[2] M.H. Oliveira *et al.*; Carbon **52**, 83-89 (2013).

HL 62.5 Wed 17:00 H17

**Graphene on cubic and hexagonal SiC: A comparative theoretical study** — Oleg Pankratov, •Stephan Hensel, Paul Götzfried, and Michel Bockstedte — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Epitaxial graphene grows on different SiC polytypes which possess distinct band gaps. We investigate the influence of polytypes on the graphene electronic spectrum employing density functional calculations with LDA and hybrid HSE functionals. We consider different buffer layer-graphene layer stackings as well as different substrate terminations.[1] We find a systematic displacement of the Dirac point relative to the valence-band edge as a function of the polytype hexagonality. The HSE values are in good agreement with available experimental results,[2,3] while LDA corroborates the trends. The Dirac point, the interface-related states, and the Fermi level follow similar polytype-dependent shifts, hence the graphene doping of the epilayer stays practically the same. For the AB stacked buffer and epilayer on Si-terminated SiC the Dirac spectrum exhibits an energy gap of 25-40 meV (depending on the polytype). On the contrary, for the AA stacking the Dirac cone remains intact. We suggest a symmetry-based analytical model which explains the origin of the gap and its absence for the AA geometry.
[1] Pankratov *et al.* Phys. Rev. B 86, 155432 (2012).
[2] Sonde *et al.*, Phys. Rev. B 80, 241406 (2009).
[3] Ristein *et al.*, Phys. Rev. Lett. 108, 246104 (2012).

HL 62.6 Wed 17:15 H17

**Phonons of graphene on SiC(0001)** — Stefan Fryska[1], Roland J. Koch[1], Felix Fromm[1], Alejandro Molina-Sánchez[2], •Ludger Wirtz[2], Martina Wanke[1,3], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg — [2]University of Luxembourg — [3]TU Chemnitz

Epitaxial graphene (EG) on SiC(0001) can be grown on a wafer scale [1] but its charge carrier mobility is considerably lower than that of graphene flakes obstained by mechanical exfoliation. A previous study [2] of the temperature dependence of the mobility suggested that it is determined by remote phonon scattering with phonons of the buffer layer at the interface between EG and SiC(0001). The buffer layer, which is identical to the $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$ reconstruction of SiC(0001), consists of a monolayer of carbon atoms in a honeycomb structure. Due to a strong interaction with the substrate, the buffer layer has destorted $\pi$-bands and does not exhibit a Dirac cone [3]. In order to learn more about the phonons of the buffer layer we have carried out a study using high-resolution electron energy loss spectrscopy (HREELS) and Raman spectroscopy, accompanied by *ab-initio* calculations. We observe strong modifications of the phonons of the buffer layer with respect to weakly interacting, quasi-free standing graphene on SiC(0001). In particular, the Kohn anomaly is quenched, which agrees with the lack of a Dirac cone. [1] K. V. Emtsev et al., Nat. Mater. **8** (2009) 203. [2] F. Speck et al., Appl. Phys. Lett. **99** (2011) 122106. [3] K. V. Emtsev et al., Phys. Rev. B **77** (2008) 155303.

HL 62.7 Wed 17:30 H17

**Intercalation of hydrogen at the graphene/Ir(111) interface** — •Thorsten Balgar, Hyunil Kim, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

Epitaxially grown graphene on an iridium crystal exhibits a well known moire pattern due to the lattice mismatch of graphene and the Ir(111) surface. This leads to a buckling of the carbon layer and a lateral modulation of the chemical reactivity towards adsorbates [1,2]. Unlike intercalated metal atoms hydrogen cannot be directly detected with surface scientists' standard analysis tool box, namely XPS or AES. In our study we have used vibrational sum frequency generation (SFG) spectroscopy to monitor the stretching vibration of hydrogen chemisorbed on graphene [3]. The results are discussed in view of the intercalation of hydrogen and the local formation of graphane-like structures.

[1] C. Busse et al., Phys. Rev. Lett. 107 (2011) 036101 [2] J. Wintterlin et al., Surf. Sci. 603 (2009) 1841 [3] Kim et al., Chem. Phys. Lett. 546 (2012) 12

HL 62.8 Wed 17:45 H17

**Decoupling of Epitaxial Graphene on Ir(111) by Oxygen Intercalation** — •Søren Ulstrup[1], Rosanna Larciprete[2], Paolo Lacovig[3], Matteo Dalmiglio[3], Marco Bianchi[1], Jens Christian Johannsen[1], Federico Mazzola[1], Liv Hornekär[1], Fabrizio Orlando[4], Alessandro Baraldi[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Sincrotrone Trieste, Trieste, Italy — [4]Physics Department and Center of Excellence for Nanostructured Materials, University of Trieste, and IOM-CNR Laboratorio TASC, Area Science Park, Trieste, Italy

Epitaxial growth of graphene on transition metal surfaces is now a well-established method for obtaining extended layers of high quality graphene. However, interactions between graphene and its metal substrate are unwanted in applications typically requiring a mechanical transfer of the graphene. Here we demonstrate a different strategy based on decoupling the graphene from an Ir(111) substrate by oxygen intercalation. More specifically, we present evidence using photoelectron spectroscopy techniques that the intercalation results in an extended layer of hole-doped quasi free-standing graphene (QFG). Analysis of the electronic self-energy near the Fermi level reveals an extremely weak electron-phonon coupling in QFG. Finally, we find that abrupt deintercalation of oxygen occurs at elevated temperatures, which is accompanied by a modest etching of the graphene lattice.

HL 62.9 Wed 18:00 H17

**Transfer-free electrical insulation of epitaxial graphene from its metal substrate** — Silvano Lizzit[1], Rosanna Larciprete[2], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[3,4], Alessandro Baraldi[3,4], Lauge Gammelgaard[5], •Lucas Barreto[6], Marco Bianchi[6], Edward Perkins[6], and Philip Hofmann[6] — [1]Sincrotrone Trieste, Italy — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Physics Department and CENMAT, University of Trieste,Italy — [4]IOM-CNR Laboratorio TASC, Trieste, Italy — [5]Capres A/S, Lyngby, Denmark — [6]Institut for Fysik og Astronomi, Interdisciplinary Nanoscience Center (iNANO), Aarhus Universitet Denmark

High-quality, large-area epitaxial graphene can be grown on metal surfaces, but its transport properties cannot be exploited because the electrical conduction is dominated by the substrate. Here we show how to insulate epitaxial graphene from the Ru(0001) surface it is grown on by a step-wise intercalation of silicon and oxygen, and the eventual formation of a $SiO_2$ layer between the graphene and the metal. The reaction steps are followed by x-ray photoemission spectroscopy. The presence of a $SiO_2$ layer should insulate the metal from the substrate. In order to verify this, lateral transport measurements were performed using a nano-scale multipoint probe technique. The resistance obtained is substantially higher than expected for a clean ruthenium surface but consistent with that expected for graphene. Moreover, the data suggest two-dimensional electronic transport, as expected for graphene.

HL 62.10 Wed 18:15 H17

**Intercalation as a route to atomically sharp graphene/ferromagnet interfaces: Structural and electronic investigations** — •Philipp Leicht, Konstantin Krausert, Lukas Zielke, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The interface between graphene (G) and the substrate plays a vital role for the electronic properties of G. Apart from direct growth of G on a small number of substrates, a variety of metals can be intercalated between G and the substrate interface [1,2] and allow for the production of G on a large number of materials. In this work, we present the investigation of Ni intercalation underneath G on Ir(111). The atomic structure and electronic properties were investigated for samples with intercalated Ni ranging from a submonolayer to few monolayers.

For Ni intercalation underneath G/Ir(111), scanning tunneling microscopy shows strongly increased moiré corrugation as well as a decreased average distance of G/Ni/Ir(111) compared to G/Ir(111). The stronger corrugation is accompanied by considerable changes in the electronic structure of the G layer. The intercalation channels including the influence of defects and diffusion of intercalants within the graphene-metal interface are discussed for the two regimes of submonolayer and multilayer intercalation.

[1] M. Sicot et al. ACS Nano 6, 151 (2012) [2] L. Huang et al. Appl. Phys. Lett. 99, 163107 (2011)

HL 62.11 Wed 18:30 H17

**Magnetism of graphene/Ir(111) intercalation systems** — •Régis Decker[1], Jens Brede[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-30355 Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungzentrum Jülich, D-52425 Jülich

The presence of intercalation compounds in graphite, i.e. impurities or layer(s) trapped between carbon sheets, can lead to changes in the transport, optical and catalytic properties compared to bulk graphite, or even to superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. Furthermore, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, we present the local structure and magnetic properties of graphene on magnetic substrates, resolved by spin-polarized STM. The magnetic substrates are obtained by the intercalation of 3d elements (Co and Fe) between graphene and the Ir(111) surface [1]. In both cases, the atomic structure of the graphene layer is dominated by a highly corrugated Moiré pattern. Within the Moiré pattern different regions are identified. Interestingly, these regions show very different electronic and magnetic signatures in the experiments. The experimental observations are compared to state-of-the-art first principles density functional theory calculations.

[1] Atomic-scale magnetism of cobalt-intercalated graphene. R. Decker et al., accepted in Phys. Rev. B (Rapid Comm.).

HL 62.12 Wed 18:45 H17

**Deuteration kinetics of the graphene** — •Alexei Nefedov[1], Alessio Paris[2], Nikolay Verbitskiy[3,11], Ying Wang[4], Alexander Fedorov[5,6], Danny Haberer[5], Martin Oetzelt[7], Luca Petaccia[8], Dmitry Usachov[6], Denis Vyalikh[6,9], Hermann Sagdev[10], Christof Woell[1], Martin Knupfer[5], Berndt Buechner[5], Lucia Calliari[2], Lada Yashina[3], Stephan Irle[4], and Alexander Grüneis[5,11] — [1]KIT, Leopoldshafen, Germany — [2]FBK-CMM, Trento, Italy — [3]MSU, Moscow, Russia — [4]Nagoya University, Nagoya, Japan — [5]IFW Dresden, Dresden, Germany — [6]St. Petersburg University, St. Petersburg, Russia — [7]BESSY II, Berlin, Germany — [8]Elettra, Trieste, Italy — [9]TU Dresden, Dresden, Germany — [10]MPI für Polymerforschung, Mainz, Germany — [11]University of Vienna, Vienna, Austria

The kinetics of the hydrogenation/deuteration reaction of graphene was studied by time-dependent x-ray photoemission spectroscopy (XPS). The graphene layer was then exposed to hydrogen or deuterium atomic gas beams, obtained by thermal cracking in a tungsten capillary at T=3000 K. After each step XPS of the C1s line was performed in order to measure H/C and D/C ratios. We have observed a strong kinetic isotope effect for the hydrogenation/deuteration reaction leading to substantially faster adsorption and higher maximum D/C ratios as compared to H/C (D/C~35% vs. H/C~25%).

HL 62.13 Wed 19:00 H17

**Intercalated thin films on Graphene/Ir(111)** — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy S Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastr. 5, D-13355 Berlin

The investigation of graphene/metal systems is interesting from fundamental as well as applications-oriented point of view. Here we report on the interaction of weakly and strongly bound intercalated metals (Cu vs. Ni) with graphene grown on Ir(111), using core and valence level photoemission spectroscopy. Studying the electronic structure of graphene in these interfaces reveals the effect of weak and strong interaction between graphene and the underlying intercalated thin film. The graphene/Ni/Ir(111) system shows a strong hybridization between the graphene $\pi$-band and the Ni 3d valence bands, which leads to the destruction of the graphene Dirac cone. The graphene/Cu/Ir(111) system, on the other hand, shows at first glance the properties of weakly bonded graphene (Dirac cone with a linear dispersion of the $\pi$-band) but with additional doping due to the donation of electrons by the intercalated Cu. Contrary to the weakly bonded scenario we observe a hybridization between the distinct Cu3d states and the graphene $\pi$-band.