TT 46: Poster Session: Graphene (joint session O/TT)

Time: Tuesday 18:15–20:30 Location: Poster A

TT 46.1 Tue 18:15 Poster A

The effects of defects and disorder on the electronic structure of graphene — •Piotr Kot[1], Jonathan Parnell[2], Sina Habibian[2], Pavel Ostrovsky[1], and Christian Ast[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada

We use a real-space nearest neighbor tight-binding model to study the effect of defects on the band dispersion of graphene. We find that defects in graphene either generally preserve the canonical band structure, or disrupt it by separating the two cones creating an "elongated" Dirac point. This second structure greatly resembles the band dispersion of experimentally measured epitaxial graphene. By using a self-consistent T-matrix approximation we find the reason why defects create two distinctly different band structures, by showing that point defects are either resonant or non-resonant in graphene. Adding all these pieces together, we conclude on the cause of "elongation" in epitaxial graphene and the nature of the electronic structure in the "elongated" region finding that this region can not be considered a gap.

TT 46.2 Tue 18:15 Poster A

Spin and charge transport in quasi-freestanding epitaxial graphene grown by CVD — •Jantje Schommartz[1,2], Alexey Kaverzin[2], Christoph Tegenkamp[1], and Bart J. van Wees[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland — [2]Physics of Nanodevices, University of Groningen, Netherlands

A promising route for the synthesis of homogeneous large-area graphene, suitable for standard device fabrication techniques, is the epitaxial growth of graphene on SiC. In the present work the growth is achieved by chemical vapor deposition (CVD) by using a hydrocarbon precursor for the carbon deposition on the Si-face of the SiC wafer. We study the quasi-freestanding epitaxial CVD graphene (CVD- QFEG) grown on 6H-SiC(0001) by contacting it with ferromagnetic Cobalt electrodes made by electron-beam lithography technique. By standard lock-in techniques we address the charge and spin transport properties independently by local and non-local measurement geometries. To the best of our knowledge, we detect for the first time spin signatures in transport measurements on CVD-QFEG. This study shows that the CVD-QFEG reveals striking differences in spin and charge transport properties compared to CVD epitaxial graphene. We attribute this to the influence of localized states arising from the buffer layer consistent with the measurements performed on epitaxial graphene grown by sublimation.

TT 46.3 Tue 18:15 Poster A

Preparation and characterization of high quality stacks of graphene/h-BN/graphite picked up by a mica substrate — •Michael Weimer[1], Tjorven Johnsen[1], Sayanti Samaddar[1], Peter Nemes-Incze[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [2]Centre of Energy Research, Institute of Technical Physics and Materials Science, Nanotechnology Department, 2D NanoFab ERC Research Group, Budapest, 1525, POB 49, Hungary

Graphene on h-BN provides a highly mobile two-dimensional electron system (2DES) which can be characterized by scanning tunneling microscopy (STM). In combination with transport experiments, a comparison of global and local properties of the sample is feasible. Such combination requires an ultra clean graphene surface and at least two electrical contacts. Therefore we present a dry and polymer free preparation technique by using a mica substrate. We exfoliate graphite on mica and subsequently pick up h-BN and graphene from a SiO_2/Si chip one after another. Shadow mask evaporation of gold provides clean contacting. Omitting wet chemical methods and polymers enables ultra clean surfaces with low impurity concentration.

TT 46.4 Tue 18:15 Poster A

Effect of the carbon 1s core hole on the polarized x-ray spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Bandstructure calculations using the WIEN2K code have been performed to study the polarized x-ray reflection spectra of highly oriented pyrolytic graphite (HOPG). Varying the amount of the included 1s core hole we find that the DFT calculations provide good agreement with experimentally obtained x-ray spectra [1]. The change of x-ray polarization upon reflection of linearly polarized synchrotron radiation can be become as huge as a birefringent rotation of polarization plane of up to 140°, and the polarization changes from linear to nearly fully circular polarization. The best calculated results are obtained for a partial core hole per excitation. The distinct contributions from the A and B sites of HOPG to the spectra are discussed as well.

Refereces: 1. C. Jansing et al, PRB 94, 045422 (2016).

This work was supported by CSF grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

TT 46.5 Tue 18:15 Poster A

Polycyclic molecules with geometrical frustration via pyrolysis on a metal — •Alexandre Artaud[1], Laurence Magaud[2], Kitti Ratter[3], Bruno Gilles[3], Valérie Guisset[2], Philippe David[2], Jose I. Martinez[4], Jose A. Martin-Gago[4], Claude Chapelier[5], and Johann Coraux[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Germany — [2]CNRS, Institut Néel, Grenoble, France — [3]Grenoble INP, SIMAP, Grenoble, France — [4]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain — [5]CEA, INAC, PHELIQS, Grenoble, France

The geometry of molecules is a key to several of their properties. In graphene fragments, electron delocalization from one carbon sublattice to the other is frustrated for molecular shapes breaking the balance of sublattices. Optical, electronic, and magnetic properties emerge in this case, but the synthesis of such molecules remains challenging.

Here, a pyrolysis reaction catalysed by the surface of rhenium is investigated using scanning tunneling microscopy and density functional theory. This reaction known to form graphene is found to also yield graphene fragments consisting of well-defined, zigzag-edged polycyclic molecules, some of which have sublattice imbalance. However, they are found in metastable configurations, which is interpreted as a kinetic rather than thermodynamic control of their formation. Hence, metastable molecules are expectedly ubiquitous in graphene growth, and deleterious to achieve perfect graphene. Pyrolysis is conversely a promising route towards molecules with sought-after properties.

TT 46.6 Tue 18:15 Poster A

Scanning Tunneling Microscopy and spectroscopy of Au islands on graphene/Rh(111) — •Anne Holtsch and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Using scanning probe techniques we investigated how graphene (gr) electronically interacts with substrates in the presence of metallic islands on top of the gr layer. In the case of rhodium as a substrate, the band structure is significantly altered with respect to freestanding graphene due to the hybridization of its d orbital with the pz orbital of gr [1]. Using scanning tunneling spectroscopy (STS) the influence of Au Islands on top of the gr was investigated. The islands were deposited by in-situ evaporation. Subsequently their relative orientation with respect to the gr lattice was observed by scanning tunneling microscopy (STM). The STS measurements on and in the vicinity of the islands show locally varying electronic properties of the system. The presence of gold induces the opening of a band gap. At the same time there is an increase in conductivity, compared to the conductivities of gold and gr. Measurements show that the increase in conductivity is restricted to that area of the islands which adjoins to the gr. In this case both gr and gold contribute to a increase of the measured tunnel current.

[1] A. Holtsch, T. Euwens, B. Uder, S. Grandthyll, F. Müller, and U. Hartmann, Surf. Sci. 668 (2018) 107.

TT 46.7 Tue 18:15 Poster A

Landau quantization in a graphene monolayer on WSe_2 and $NbSe_2$ — •Felix Förschner[1], Lena Stoppel[1], Fabian Paschke[1], Julia Tesch[1], Yuriy Dedkov[2,1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Deutschland — [2]Department of Physics, Shanghai University, 200444 Shanghai, China

By depositing graphene on transition metal dichalcogenides (TMDs), it is possible to alter the electronic properties of graphene [1]. Here we focus on the fabrication of graphene on WSe_2 and $NbSe_2$, which was successfully performed by an adapted wet chemical transfer process. By means of low-temperature scanning tunneling microscopy we investigate the atomic structure of graphene and observe different Moiré structures indicating a successful transfer of graphene onto the TMD. In an external magnetic field, Landau level sequences are observed giving access to the electronic properties of graphene, i.e. doping level, Fermi velocity etc. Detailed analysis of the obtained tunneling spectra shows that each Landau level is split into subpeaks, where the pronounced splitting strength grows with increasing magnetic field. The magnitude of the observed splitting indicates an enhanced spin-orbit interaction strength in graphene due to the presence of the TMD substrate.

[1] Z. Wang *et al.*, Nature Comm. **6**, 8339 (2015).

TT 46.8 Tue 18:15 Poster A

Dislocations in bilayer graphene — •Florian Wullschläger, Konstantin Weber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Dislocations, i.e. one-dimensional line defects, are the main carriers of plastic deformation in 3D crystalline solids. In a recent TEM study it was shown that dislocations even exist in materials as thin as two graphene layers [1]. Using atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [2] we show that the properties of dislocations in quasi-2D crystals differ significantly from their 3D counterparts. The step components of the dislocations give rise to a pronounced buckling of the bilayer in order to release strain energy. All dislocations split into equally-spaced partials due to the absence of a stacking fault energy, a peculiar property of bilayer graphene. Finally, in 2D materials the strain energy induced by a dislocation does not diverge with sample size as in 3D, but remains finite. In addition to this structural characterization of 2D dislocations we will show first results on how dislocations move in bilayer graphene and how they are pinned at lattice defects.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, Nature **505** (2014) 533.
[2] A. Kolmogorov, V. Crespi, Phys. Rev. B **71** (2005) 235415.

TT 46.9 Tue 18:15 Poster A

Microscopic investigations of graphene-nickel interactions — •Philip Schädlich, Florian Speck, Adrian Schütze, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz

In order to realize possible applications of graphene in electronics, it is important to understand the properties of graphene - metal contact interfaces. In this study we investigate the impact of nickel as possible contact material on the underlying graphene.

Graphene samples are grown by sublimation of Si atoms from a 6H-SiC(0001) substrate in Ar atmosphere at ambient pressure [1]. The local graphene coverage is probed by photoemission electron microscopy as well as low-energy electron microscopy (LEEM) and reflectivity (LEER) spectra. The deposition process of nickel is monitored *in-situ* via LEEM. After deposition, LEER spectra indicate a change of the work function in the covered areas while the characteristic interlayer states [2] stay unchanged. The morphology of the deposited nickel layer is revealed by atomic force microscopy, while the thickness was determined by x-ray photoemission spectroscopy. Angle-resolved photoemission spectroscopy confirms an unchanged electronic band structure with the Dirac point located 0.4 eV below the Fermi energy, which is close to values found for bare monolayer graphene on the 6H-SiC(0001) surface.

[1] K. V. Emtsev et al., Nature Materials 8, 203 (2009).
[2] N. Srivastava et al. Phys. Rev. B 87, 245414 (2013).

TT 46.10 Tue 18:15 Poster A

Development of a high-dimensional neural network potential for hydrogen atoms at graphene. — •Sebastian Wille[1,2], Marvin Kammler[2], Martín L. Paleico[3], Jörg Behler[3], Alec M. Wodtke[1,2], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

To fully understand atom-surface interactions, the availability of an accurate full-dimensional potential energy surface (PES) is crucial. High-dimensional neural network potentials have been shown to provide very accurate PESs for a wide range of systems. Here, we develop a neural network potential for H-atom scattering from a graphene sheet. We fit the potential to density functional theory energies calculated on-the-fly in *ab initio* molecular dynamics simulations. We find that the procedure can reliably describe H at graphene, which makes it possible to effectively simulate the scattering for this system in a large range of incidence conditions.

TT 46.11 Tue 18:15 Poster A

Influence of atomic-scale dopants on the transport properties of graphene on SiC — •Anna Sinterhauf[1,2], Philip Willke[1], Georg Traeger[1], Davood Momeni Pakdehi[3], Klaus Pierz[3], Hans Werner Schumacher[3], Hans Hofsäss[4], and Martin Wenderoth[1,2] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]International Center for Advanced Studies of Energy Conversion (ICASEC), Universität Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt Braunschweig, Germany — [4]II. Physikalisches Institut, Universität Göttingen, Germany

Tailoring the electronic structure of graphene by substitutional doping often additionally changes its transport properties. In order to study the impact of atomic-scale dopants on electron transport, graphene samples were prepared by polymer-assisted sublimation growth (PASG) [1] and doped with nitrogen atoms by low energy ion beam implantation [2]. Using highly resolved scanning tunneling microscopy and potentiometry, we determined the dopant density as well as the local sheet resistance on the nanometer scale. Moreover, the defect resistance at substrate steps was evaluated. Subsequently, the mobility and the mean free path length were estimated and compared for pristine and nitrogen doped PASG graphene. Furthermore, we were able to quantify the impact of nitrogen dopants on the charge transport, which introduce an additional short-range scattering process along with long-range Coulomb scattering. [1] Kruskopf et al., 2D Materials 3, 041002, 2016 [2] Willke et al., Nano Lett. 15(8), 2015

TT 46.12 Tue 18:15 Poster A

Variation of the local transport properties of epitaxial graphene caused by the stacking order of 6H-SiC — •Georg Traeger[1], Anna Sinterhauf[1,2], Davood Momeni Pakdehi[3], Philip Schädlich[5], Florian Speck[5], Johannes Aprojanz[4,5], Thomas Seyller[5], Hans-Werner Schumacher[3], Christoph Tegenkamp[4,5], Klaus Pierz[3], and Martin Wenderoth[1,2] — [1]IV. Physical Institute, University of Göttingen, Göttingen, Germany — [2]Internatonal Center for Advanced Studies of Energy Conversion (ICASEC), University of Göttingen, Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Institute for Solid State Physics, University of Hannover, Hannoner, Germany — [5]Institute of Physics, Chemnitz, Chemnitz, Germany

We present a scanning tunneling potentiometer (STP) study on graphene on silicon carbide (6H-SiC(0001)) grown by polymer assisted sublimation growth (PASG). The high homogeneity of the buffer layer, grown by PASG allows for an investigation of the substrate graphene interaction. [1] Highly resolved STP measurements revealed two distinct sheet resistances, which occur in a characteristic pattern. We identified this pattern with the 6H stacking sequence of the substrate and assigned the graphene terraces to different substrate terminations. Park et al. found that these terminations have different polarization charges [2]. According to this findings, we attribute the termination with the highest polarization charge to the graphene sheet with the highest conductivity.

[1] Pakdehi et al., Submitted [2] Park et al., Phys. Rev. B, 1995

TT 46.13 Tue 18:15 Poster A

Ru - mediated growth of graphene on SiC for radiation sensing application — •Rajesh Kumar Chellappan, Simon Cooil, Marina Jorge, Håkon Røst, and Justin Wells — Center for Quantum Spintronics, Norwegian University of Science and Technology, Norway

Graphene has been proposed as a suitable candidate for photo/radiation sensors primarily because of its exceptional electronic properties. However, this advantage has been difficult to realize because of the problems associated with the preparation of high quality graphene on dielectric/semiconductor substrates. Therefore, this study focuses on addressing epitaxial ruthenium mediated graphene growth on silicon carbide and the subsequent interface oxidation using soft X-ray photoemission spectroscopy (SXPS). The growth of graphene and formation of ruthenium silicide was investigated by systematic annealing of ruthenium (~1nm) deposited on silicon carbide samples in vacuum at temperatures ranging from 450°C to 700°C. The interlayer oxidation was achieved by exposing the sample at 460°C to oxygen partial pressure of 9.5*10-7 mbar for 1 hour to form a graphene/dielectric/silicon carbide device structure.