# O 7: Graphene I: Structure and Dynamics

Time: Monday 10:30–13:30 Location: H24

O 7.1 Mon 10:30 H24

**The electronic structure of graphene superlattices revisited** — •Pilkwang Kim[1] and Cheol-Hwan Park[2] — [1]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul, Korea

We present the calculated electronic structure of graphene superlattices, which are graphenes under lateral, periodic potential. Previous studies on a graphene superlattice [1-3] have reported anisotropic group velocity renormalization, emergence of new zero-energy points, conductance resonance, etc. However, several features manifested in the electronic structure obtained from our numerical calculations, e.g., the movement of the Dirac points in momentum space, cannot be explained by the theories introduced in those studies. In this presentation, we discuss the reason why there are features in the electronic structure of graphene superlattices that were not captured by previous theories. We also discuss electronic structure obtained by using first- and higher-order perturbation calculations.

1.Park, C.-H., Yang, L., Son, Y.-W., Cohen, M. L. & Louie, S. G. New generation of massless Dirac fermions in graphene under external periodic potentials. Phys. Rev. Lett. 101, 126804 (2008). 2.Barbier, M., Vasilopoulos, P. & Peeters, F. M. Dirac electrons in a Kronig-Penney potential: Dispersion relation and transmission periodic in the strength of the barriers. Phys. Rev. B 80, 205415 (2009). 3.Brey, L. & Fertig, H. A. Emerging Zero Modes for Graphene in a Periodic Potential. Phys. Rev. Lett. 103, 046809 (2009).

O 7.2 Mon 10:45 H24

**Confinement effects in quasiparticle interference on epitaxial graphene nanoflakes** — •Julia Tesch[1], Philipp Leicht[1], Felix Blumenschein[1], Tomas Löfwander[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

In the search for suitable materials to be used in nanoscale electronic devices, graphene quantum dots, ribbons and flakes have attracted increased attention amongst researchers, as they allow for a combination of graphene's linear electronic dispersion relation with interesting physical phenomena arising from the size quantization of the structures.

We present a comprehensive study of epitaxial graphene nanoflakes on noble metal surfaces by means of low-temperature scanning tuneling microscopy and spectroscopy. The analysis of quasiparticle interference patterns produced by elastic scattering at defects allows for a clear identification of graphene-related contributions visible as ringlike *inter-* and *intravalley* features within the Fourier transform images [1]. Lateral electronic confinement within these elongated flakes gives rise to additional scattering intensity related to transitions between the flake's transverse modes [2]. Additionally, we discuss the influence of edge configuration, lattice symmetry breaking and quasiparticle lifetime on the scattering, by comparison of the experimental results with tight-binding calculations of realistic graphene nanoflakes.

[1] P. Leicht *et al.*, ACS Nano **8**, 3735 (2014); [2] A. Bergvall *et al.*, Phys. Rev. B **87**, 205431 (2013).

O 7.3 Mon 11:00 H24

**Electron interference in ballistic graphene nanoconstrictions** — •Johannes Aprojanz[1], Jens Baringhaus[1], Mikkel Settnes[2], Stephen Power[2], Anti-Pekka Jauho[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

Graphene nanoconstrictions (GNCs) are a central building block of future carbon electronic devices. However, the synthesis of constrictions with well-defined edges is challenging. Here, we use the tip of a scanning tunneling microscope (STM) for the local etching of graphene, which allows to define GNCs with variable dimensions of down to 1 nm. The GNCs are etched into fully ballistic graphene nanoribbons hosted on the sidewalls of SiC mesa structures [1]. Due to the highly precise etching technique as well as the exceptional electronic quality of the graphene (e.g. mean free path $> 10\ \mu$m), this system is ideal to study coherent transport phenomena. Therefore, the transport characteristics of constrictions with various dimensions are recorded by means of a variable temperature 4-tip-STM. Electron interference at the abrupt graphene interfaces gives rise to characteristic conductance peaks and transport gaps. Their appearance is described by a tight-binding and recursive Green's function approach which especially highlights the robustness of the resonances features against temperature as well as disorder.

[1] Baringhaus et al., Nature **506**, 349 (2014)

O 7.4 Mon 11:15 H24

**Graphene on Ru(0001) as a playground for the studies of the graphene-metal interaction** — Elena Voloshina[1], Nikolai Berdunov[2], and •Yuriy Dedkov[2,3] — [1]HU Berlin, Germany — [2]SPECS GmbH, Germany — [3]IHP Frankfurt (Oder), Germany

We employ a combination of surface science methods (ARPES, STM/STS, AFM) and DFT calculations for the studies of the lattice mismatched graphene-Ru interface. Our results demonstrate a site-selective interaction (*strong* vs *weak*) between graphene and metal in the moiré lattice. In these studies we show that graphene-*hills* in this structure can be used as an array of electro-mechanical elastic nano-resonantors with very high resonance frequency (in the THz range). On the next step we modify the graphene-Ru interaction via intercalation. Here the scanning probe microscopy and spectroscopy were used to study the crystallographic structure and electronic properties of the uniform free-standing graphene layers obtained by intercalation of oxygen monolayer in the *strongly* bonded graphene/Ru(0001) interface. Spectroscopic data show that such graphene layer is heavily $p$-doped with the Dirac point located at 552 meV above the Fermi level, that corroborates our ARPES data. Experimental data are understood within DFT and the observed effects are in good agreement with the theoretical data.

**Invited Talk** O 7.5 Mon 11:30 H24

**Direct view on non-equilibrium carriers in graphene with time-resolved ARPES** — •Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The linear band structure of graphene bares great potential for optoelectronic applications ranging from Terahertz lasing to efficient light harvesting. We explore the response of the Dirac carriers in lightly hole-doped epitaxial graphene samples to three different excitation schemes: interband transitions for $\hbar\omega_{\mathrm{pump}} > 2\mu_{\mathrm{e}}$, free carrier absorption for $\hbar\omega_{\mathrm{pump}} < 2\mu_{\mathrm{e}}$, and resonant phonon excitation for $\hbar\omega_{\mathrm{pump}} = 200\,\mathrm{meV}$. Time- and angle-resolved photoemission spectroscopy (tr-ARPES) allows us to map the transient population of the Dirac cone in momentum space over a large energy window of several electron Volts down to arbitrarily small excitation energies.

We find a short-lived population-inverted state for interband excitation [1], a simple metallic relaxation behaviour for free carrier absorption [1], and indications for a transient enhancement of the electron-phonon coupling constant when resonantly driving the in-plane phonon in bilayer graphene [2]. Furthermore, by improving the temporal resolution to $\sim$10 fs, we were able to identify impact ionization as the primary thermalization channel within the first $\sim$25 fs [3].

[1] Gierz et al., Nature Materials 12, 1119 (2013)
[2] Gierz et al., PRL 114, 125503 (2015)
[3] Gierz et al., PRL 115, 086803 (2015)

O 7.6 Mon 12:00 H24

**Electronic properties of ytterbium interaction with graphene on Ir(111)** — Hendrik Vita[1], •Stefan Böttcher[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

The intercalation of metals in between graphene monolayers and a substrate is interesting from several points of view, for example in order to understand the effect of symmetry lowering in the interaction of the metal states with the specific graphene $\pi$ bands in the region of the "Dirac cone". Here we present a study of the intercalation of a rare earth metal, Yb, in between graphene and Ir(111). Ytterbium exhibits an s-type valence band, making it possible to compare the electronic structure to the widely studied cases of alkali metals used as intercalates in graphene intercalation compounds. Using core level spectroscopy we follow the deposition of Yb and the evolution of the intercalated phase. LEED studies show that the structural arrangement of the intercalated Yb thin film leads to a $(\sqrt{3}\times\sqrt{3})$R30° phase. Angle-resolved photoemission reveals that the interaction between the metal states and the graphene $\pi$ band near the K point induces an extremely strong n-type doping. Hybridization-induced band gaps open in the $\pi$ band at binding energies of 0.3 eV and 1.6 eV due to the interaction with the strongly localized metal $4f$ states. We compare our data with other weakly and strongly interacting intercalated metal layers.

O 7.7 Mon 12:15 H24

**Plasma-assisted CVD graphene synthesis and characterization on nickel substrates** — •Patricia Pop-Ghe, Lisa Krückemeier, Nicolas Wöhrl, and Volker Buck — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr, 1, 47057 Duisburg, Germany

This work presents the synthesis of graphene by plasma-assisted chemical vapour deposition on polycrystalline nickel foils. It is initiated by the comparison of the mechanisms in CVD and plasma-assisted CVD on a nickel substrate and focusses on the development of a growth model for both sides of the substrate within the experimental results. In detail, the differences in graphene growth at the front and at the back side of the substrate are investigated and correlated to specific influence factors. It is shown that growth mode as well as expansion and quality of graphene sheets can be adjusted by process temperature and time respectively since carbon solubility and diffusion in nickel both hold strong temperature and time dependencies. The strong time dependance of graphene growth is further indicative of a reconstructional nature of graphene formation, which is further discussed in the developed growth model. In addition the influence of the substrate is investigated by comparing results from graphene growth on polycrystalline nickel foils and nickel single crystal(111) substrates, as well as graphene on nickel (synthesized graphene) and silicon dioxide substrates (transferred graphene). Raman mappings are demonstrated to confirm the quality of the synthesized graphene.

O 7.8 Mon 12:30 H24

**Determination of the optical constants of graphene at the carbon K-edge by transmission spectroscopy** — •Christine Jansing[1], Hans-Christoph Mertins[1], Andreas Gaupp[1], Andrey Sokolov[2], Markus Gilbert[1], Andreas Schümmer[1], Hud Wahab[3], Heiko Timmers[3], Suk-Ho Choi[4], and Dominik Legut[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]Kyung Hee University, Yongin 446-701, Korea — [5]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic

The transmission of linearly polarized synchrotron radiation through quasi-free-standing graphene, supported by a Si3N4-membrane, has been measured across the carbon K-edge. From the measured absorption spectrum, that represents the imaginary part, the real part of the refractive index has been extracted via a Kramers-Kronig transformation. Based on these detailed optical parameters, reflection spectra have been simulated for linearly polarized soft x-ray light incident on graphene-metal systems. Importantly, the simulations include the interference of light reflected from graphene and from light reflected from the metallic substrate, respectively. In addition the optical constants are compared to the ones obtained by various density function theory calculations using single-electron framework as well as the more complex many-body approaches to the electronic structure of free-standing graphene.

O 7.9 Mon 12:45 H24

**Origins of contact resistance in graphene-metal edge-contacts** — •Bernhard Kretz[1], Christian Søndergaard Pedersen[2], Daniele Stradi[2], Aran Garcia-Lekue[1,3], and Mads Brandbyge[2] — [1]Donostia International Physics Center, E-20018 San Sebastian, Spain — [2]Center for Nanostructured Graphene, DTU Nanotech, Tech. Uni. of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

The transport properties of graphene-metal contacts play an important role in the design of graphene-based devices. Recent studies demonstrate the advantages of the edge-contact geometry over conventional surface contacts.[1,2] However, significantly different conclusions are reached regarding the influence of the metal on the conductance properties of edge-contacts: while simulations indicate that the contact resistance is of the same order of magnitude for different metals,[2] experiments reveal a strong metal-dependence.[1] The possible origins of these discrepancies are explored by studying the transport properties of graphene edge-contacts with different metals, different edge conformations, terminations and adsorption distances. We employ a density functional theory (DFT) based non-equilibrium Green-function (NEGF) approach, using the TranSIESTA code. Our results will offer insights towards a better understanding of the conductance properties of graphene-metal contacts deviating from ideal interfaces.

[1] Wang et al. Science 342, 2013; Chu et al. ACS Nano 8, 2014

[2] Matsuda et al., J. Phys. Chem. C 114, 2010

O 7.10 Mon 13:00 H24

**Magnetically confined quantum dots in graphene revealed by scanning tunneling spectroscopy** — •Nils Freitag[1], Peter Nemes-Incze[1], Larisa Chizova[2], Colin R. Woods[3], Roman V. Gorbachev[3], Yang Cao[3], Andre K. Geim[3], Kostya S. Novoselov[3], Florian Libisch[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen, Otto-Blumenthal Street, 52074 Aachen, Germany — [2]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria — [3]School of Physics & Astronomy, University of Manchester, Manchester, United Kingdom

Confining graphene's chiral massless charge carriers by carving out nano-structures to circumvent Klein-tunneling suffers from disordered edges, impeding the control of the quasi-relativistic particles. Here, we use the electrostatic potential of an STM tip in combination with an homogeneous magnetic field to confine electrons in graphene without edges[1]. The confinement becomes visible as a fourfold charging sequence at B>2T, as expected from valley and spin degeneracy. Up to 40 charging peaks are observed in the hole and electron sector with charging energies of 5-10meV. Characteristic spatial charging patterns created by potential modulations of the commensurate G on BN are found[2].

[1] G. Giavaras and F. Nori, PRB 85, 165446 (2012)

[2] C. R. Woods et al., Nat. Phys. 10(6), 451-456 (2014)

O 7.11 Mon 13:15 H24

**Controling intramolecular Hydrogen-transfer by Gate-tunable STM** — •Shai Mangel[1], Christian Dette[1], Katharina Polyudov[1], Paul Punke[1], Roberto Urcuyo[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The atomic level control of the electron transport has important advantages for many applications, such as molecular electronics, solar cells and sensors. Electron transport properties can be controlled by the intramolecular reaction which reshape the electronic configuration without any significant change in the conformation. The STM-induced tautomerization, i.e the interconversion between two isomers due to the migration of Hydrogen, was observed in the form of telegraphic noise. Several methods to control the intramolecular Hydrogen-transfer by changing the chemical environment of the molecule have been developed, such as locating adatoms or introducing defects. However, these affect the molecules only in the nm range. In this work, using the gate-tunable STM, we demonstrate a global control of the chemical environment of the substrate which results in the changing of the switching rate of the Hydrogen-transfer. The system we have used is a molecular network of phthalocyanine on graphene. Understanding and controlling the influence of the field-effect on the molecules, will be crucial for the construction of future molecular devices for energy and information usages.