O 94: Graphene: Electronic Properties, Structure and Substrate Interaction II

Time: Thursday 15:00–18:15   Location: TRE Ma

O 94.1   Thu 15:00   TRE Ma
Microscopic investigations of graphene grown on copper foil
— •Philip Schädlich[1], Florian Speck[1], Julia Krone[1], Patrick
Herlinger[2], Pranoti Kshirsagar[2], Martina Wanke[1], Jurgen
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Graphene grown by CVD on polycrystalline copper foil is investigated
by PEEM, LEEM, LEED and STM. LEED indicates that the flakes
consist of rotated domains as well as twisted bilayer areas. The twist
between two graphene layers grown on top of each other leads to the
formation of periodic Moiré superstructures, which were observed by
STM. In addition, the formation of surface facets on the copper foil
gives rise to a stripe pattern in PEEM and LEEM, and a displaced
LEED pattern, which can be attributed to the inclined terraces of the
faceted surface by dark field LEEM. Inclination angles between facets
have been determined by energy dependent LEED and are comparable
with literature reports [1, 2]. AFM and STM confirm the results of
the faceted surface obtained by LEEM.
[1] S. Nie, et al., New J. Phys. **14**, 093028 (2012).
[2] J. Kraus, et al., Carbon **64**, 377 (2013).

O 94.2   Thu 15:15   TRE Ma
**Local electronic properties of the graphene-protected giant
Rashba-split BiAg$_2$ surface** — •Julia Tesch[1], Milan Jubitz[1],
Elena Voloshina[2], Yuriy Dedkov[1], and Mikhail Fonin[1] —
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In search of future spintronic devices, combined systems of graphene
and strongly Rashba-split surfaces, such as the heavy post-transition
and noble metal surface alloy BiAg$_2$, have become of particular inter-
est.

Following a detailed discussion of the challenging yet well repro-
ducible sample fabrication technique that allows us to fine tune the
properties of the resulting system, we present a comprehensive study
of the gr/BiAg$_2$ structure by means of scanning tunnelling microscopy
as well as spectroscopy supported by density functional theory calcula-
tions. Besides the persistent relativistic nature of graphene charge car-
riers upon adsorption, we report on a downward shift of the preserved
BiAg$_2$ surface state. This peculiar phenomenon can be explained by
an inward relaxation of Bi atoms into the underlying thick Ag layer
and thus a subsequent delocalisation of the surface state wavefunc-
tion. Despite the close proximity of the giant Rashba-split surface to
graphene, no spin splitting has been observed in graphene in both ex-
periment and theory, while the spin-texture of BiAg$_2$ remains intact
protected by graphene adsorption making this system a promising can-
didate for spintronic applications.

O 94.3   Thu 15:30   TRE Ma
**Controlling intramolecular hydrogen-transfer by electrostatic
doping using gate-tunable STM** — •Shai Mangel[1], Chris-
tian 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
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Electron transport properties can be controlled by intramolecular re-
actions that reshape the electronic configuration without changing the
conformation. A prominent example is tautomerization, i.e. the inter-
conversion between two isomers due to migration of hydrogen, which
can be induced by STM. Several methods to control the tautomer-
ization reaction were developed, such as depositing adatoms or using
thermal and photoinduced excitation. However, those methods are
usually limited in their spatial range and not always reversible. In this
work, we demonstrate a global control of the electron density surround-
ing H$_2$-phthalocyanine on graphene/SiO$_2$/Si. By using a gate-tunable
STM, we electrostatically doped the graphene substrate altering the
chemical potential in the molecules surrounding, which results in up
to 60% decrease of the tautomeric switching rate. This reduction is
assigned to an increase in the energetic barrier of the tautomeriza-

tion reaction. Understanding and controlling the electric field-effect
on molecules via modification of the chemical potential of graphene is
critical for designing future molecular electronic devices.

O 94.4   Thu 15:45   TRE Ma
**Structure of pristine and hBN-embedded graphene quantum
dots on Ir(111)** — •Jiaqi Cai[1], Caio Silva[1,2], Wouter Jolie[2],
Ferdinand Farwick zum Hagen[2], Christoph Schlueter[3], Tien-
Lin Lee[3], and Carsten Busse[1,2] — [1]Institut für Materialphysik,
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Nanometer-sized graphene flakes (graphene quantum dots, GQDs) pro-
vide a playground for the confinement of Dirac electrons [1]. On
Ir(111), these GQDs are dome-shaped, with their edges bend towards
and strongly bond to Ir surface atoms [2]. We prepare GQDs with an
average size of 2 nm, and explore the details of the varying graphene-
substrate interaction with the x-ray standing wave technique. We pre-
cisely measure the bond distances of the C atoms at the edges as well
as in the interior of the GQDs.

In order to stabilize these graphene nanostructures and to reach a
well-defined edge termination, we embedded the GQDs in hexagonal
boron nitride (hBN). We investigate the structural changes caused by
the embedding, especially at the graphene-hBN interface, where pecu-
liar electronic effects, such as half-metallicity are predicted [3]. The
GQDs edges remain strongly bonded to the substrate, and the interface
is comprised of both N-C and B-C bonds.
[1] W. Jolie et al., Phys. Rev. B 89, 155435 (2014).
[2] P. Lacovig et al., Phys. Rev. Lett. 103, 166101 (2009).
[3] S. Dutta et al., Phys. Rev. Lett. 102, 096601 (2009).

O 94.5   Thu 16:00   TRE Ma
**Investigation of Graphene using Simultaneous Scanning Tun-
neling/Atomic Force Microscopy** — •Majid Fazeli Jadidi and
Hakan Özgür Özer — Istanbul Technical University, Istanbul,
Turkey

We investigated graphene layers grown on Cu foils using simul-
taneous Scanning Tunneling Microscopy/Atomic Force Microscopy
(STM/AFM). Atomic resolution images of the surface were obtained in
many channels such as STM topography, oscillation amplitude, force,
tunnel barrier height and phase shift. The simultaneous acquisition of
multiple channels allows us to compare images at every pixel, which in
turn sheds light on the contrast mechanisms in probe microscopy. In
HOPG or multilayer graphene, due to the shift between two successive
layers, 3 atoms of the hexagon have an atom underneath (alpha (A)
site) whereas the other 3 don't have (beta (B) site). Hence, three main
atomic structures at the surface are A and B atoms and hollow sites.
In STM images B atoms appear higher due to the dominance of their
electronic structure over A site atoms. In the oscillation amplitude
images which is a measure of the interaction stiffness[1], the brighter
spots match with the A sites. The oscillation amplitude throughout
the entire image is well below the free amplitude which suggests a very
high positive interaction stiffness. This observation is supported also
by the Force-distance spectroscopy which is simultaneously acquired
with all such acquisition channels.
[1] A. Oral, R. A. Grimble, H. Ö. Özer, P. M. Hoffmann, and J. B.
Pethica, Appl. Phys. Lett. 79, 1915 (2001).

O 94.6   Thu 16:15   TRE Ma
Strong electron-phonon coupling in the σ band of graphene
— Federico Mazzola[1], Thomas Frederiksen[2], Thiagarajan
Balasubramanian[3], Philip Hofmann[4], •Bo Hellsing[5], and
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First-principles studies of the electron-phonon coupling in graphene
predict a high coupling strength for the σ band with values of the di-
mensionless mass-enhancement parameter λ up to 0.9. Near the top
of the σ band λ is found to be ≈ 0.7. This value is consistent with the
observed kink in the σ band dispersion near the $\bar{\Gamma}$-point in the Bril-

lion zone. The calculations show that the electron-phonon coupling is driven primarily by the optical LO and TO phonon modes in graphene. The photoemission intensity from the σ band is strongly suppressed near the $\bar{\Gamma}$-point due to sublattice interference effects. These effects are removed by taking data in the neighbouring Brioullin zone. By this we have been able to disentangle the influence of sublattice interference and electron-phonon coupling. A rigorous analysis of the experimentally determined complex self-energy further supports the assignment of the observed kink to strong electron-phonon coupling and yields $\lambda \approx$ 0.6, in excellent agreement with the calculations.

O 94.7   Thu 16:30   TRE Ma

Imaging Anisotropic Carrier Dynamics in Graphene —
●Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Hubertus Bromberger[1], Razvan Krause[1], Ameer Al-Temimy[2], Camilla Coletti[2], Andrea Cavalleri[1,3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy — [3]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Photo-excitation of graphene transfers electrons from the valence band to the conduction band in a direct interband transition. The initial distribution of holes and electrons is known to be anisotropic with nodes along the direction of the light polarization. We use time- and angle-resolved photoemission spectroscopy to image the initially anisotropic carrier distribution on constant energy cuts through the Dirac cone and follow its relaxation as a function of pump-probe time delay. We find that ultrafast collinear electron-electron scattering rapidly redistributes the energy among the carriers and establishes a momentum-dependent electronic temperature on time scales short compared to our experimental resolution. Momentum relaxation occurs mainly through optical phonon emission within approximately 100 femtoseconds determined from the time it takes for the electron distribution to become isotropic. Our measurements provide a complete picture of the ultrafast thermalization dynamics in photo-excited graphene.

O 94.8   Thu 16:45   TRE Ma

Quantifying electronic band interactions in van der Waals materials using angle-resolved reflected-electron spectroscopy —
●Johannes Jobst[1,2], Alexander J. H. van der Torren[1], Eugene E. Krasovskii[3], Jesse Balgley[2], Cory R. Dean[2], Rudolf M. Tromp[4,1], and Sense Jan van der Molen[1] — [1]Leiden Institute of Physics, Leiden University, The Netherlands — [2]Department of Physics, Columbia University, New York, USA — [3]Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian/Donostia, Spain — [4]IBM T.J. Watson Research Center, Yorktown Heights, USA

High electron mobility is one of graphene's key properties, exploited for applications and fundamental research alike. Highest mobility values are found in heterostructures of graphene and hexagonal boron nitride, which consequently are widely used. However, surprisingly little is known about the interaction between the electronic states of these layered systems. Rather pragmatically, it is assumed that these do not couple significantly. Here we study the unoccupied band structure of graphite, boron nitride and their heterostructures using angle- resolved reflected-electron spectroscopy. We demonstrate that graphene and boron nitride bands do not interact over a wide energy range, despite their very similar dispersions. The method we use can be generally applied to study interactions in van der Waals systems, that is, artificial stacks of layered materials. With this we can quantitatively understand the 'chemistry of layers' by which novel materials are created via electronic coupling between the layers they are composed of.

O 94.9   Thu 17:00   TRE Ma

Magneto-optic effects of graphene at the carbon 1s edge on metallic substrates - theory and experiment —
●Dominik Legut[1], Peter M. Oppeneer[2], Christine Jansing[3], Markus Gilbert[3], Andreas Gaupp[3], Hans-Christoph Mertins[3], Andrey Sokolov[4], Suk-Ho Choi[5], Hud Wahab[6], and Heiko Timmers[6] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [3]FH Münster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [4]HZB, Albert Einstein Str. 15, D-12489 Berlin, Germany — [5]Dept. of Applied Physics, Kyung Hee University, Korea — [6]Univ. of New South Wales Canberra, Australia

The optical properties at the carbon 1s of the free standing graphene utilizing the electronic structure models are calculated from first principles. For its better description the core-hole quasiparticle is taken into account. One can model it by the so-called Slater transition state employing the supercell calculation with partial hole on one of the carbon atoms with the electron charge distributed over the valence states. Another approach is to solve Bethe-Salpeter equations for the many-body electronic effects. The latter approach clearly identify the excitonic features of π- and σ-excitations of graphene. Next, optical response of the graphene on metallic substrate (Cu, Ni, and Co) is calculated and the degree of the hybridization between the p_z and d-states is determined, together with the identification of the magnetic moments. Next, using multilayerd optical code the T-MOKE and XMCD spectra are determined and compared with recently recorded data.

O 94.10   Thu 17:15   TRE Ma

Bottom-up synthesis of graphene nanomembranes with tunable porosity —
●Christof Neumann[1], Michael Mohn[2], Matthias Füser[3], David Kaiser[1], Ute Kaiser[2], Andreas Terfort[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm — [3]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt

The potential of 2D materials like carbon or graphene nanomembranes [1] for separation or ultrafiltration applications is based on the unique features of these novel nanomaterials having pore sizes suitable for molecular sieving and negligible thicknesses compared to the molecular mean free paths or even below. Here we present a versatile method for tuning the properties of graphene nanomembranes by conversion of 4-(1H-pyrrol-1-yl)thiophenol, 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol and 4-(pyrimidin-2-yl)phenylthiol self-assembled monolayers (SAMs) on polycrystalline copper foils into carbon nanomembranes (CNMs) via electron induced crosslinking and their further pyrolytic transformation into the nanoporous graphene monolayers. We characterize the resulting SAMs, CNMs and graphene-nanomembranes by different complementary techniques including X-ray photoelectron (XPS) and Raman spectroscopy, atomic force (AFM), helium ion (HIM) and high-resolution transmission electron microscopy (HRTEM) as well as by electric transport measurements. [1] A. Turchanin and A. Gölzhäuser, Adv. Mater. 28, 5075 (2016)

O 94.11   Thu 17:30   TRE Ma

tracking electron dynamics in graphene and TMDCs —
●Cephise Cacho — Artemis - Central Laser Facility, Didcot, UK

Novel quantum materials such as graphene and transition metal dichalcogenides (TMDC) are attracting vast interest particularly for their application in spintronic and optoelectronic devices. Their properties are intrinsically governed by the large momentum electrons (at the Brillouin zone K-point). In order to eject such electrons in vacuum and observe their dynamics, a high energy (>20 eV) photon source is required as well as ultrashort pulse duration. High Harmonic Generation source [1] combined to an Angle-Resolved PhotoEmission Spectroscopy (ARPES) end-station is a powerful tool to observe such electron dynamics. After an introduction on ARPES and experimental concepts, I will present an overview of recent time-resolved ARPES studies [2-6] performed at the Artemis facility.

Single-layers of MoS2, WS2 and bulk WSe2 were resonantly pumped across the band gap at the K point. Monitoring the valence/conduction bands population reveals the band dynamics during excitation. Furthermore the intervalley scattering is explored by exciting the surface with circularly polarized light.

References 1. F. Frassetto et al., Optics Express 19, 19169 (2011) 2. E. Pomarico et al., arXiv:1607.02314 (2016) 3. A. Grubišić Čabo et al., Nano Lett. 15, 5883 (2015) 4. S. Ulstrup et al., ACS Nano 10, 6315 (2016) 5. S. Ulstrup et al., arXiv:1608.06023 (2016) 6. R. Bertoni et al., arXiv:1606.03218 (2016)

O 94.12   Thu 17:45   TRE Ma

Phase diagram of a graphene bilayer in the zero-energy Landau level —
●Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques (LPTMS), Université Paris-Sud, 91405 Orsay, France

We theoretically investigate the ground state structure of bilayer graphene (BLG) in the quantum Hall regime. In BLG, the zero energy states carry, besides the real spin, two pseudospin degrees of freedom:

a valley isospin and a Landau level (n = 0, n = 1) isospin. This peculiar property leads to an octet of states that is eightfold degenerate in the absence of any symmetry breaking and can be treated in the frame of quantum Hall ferromagnetism. If this SU(8) symmetry is indeed broken, an extraordinary rich phase structure emerges, with each phase characterized by a different spin and isospin configuration. Recent experiments have revealed a plethora of transitions upon variation of the strength of an applied magnetic or electric field. We start from a four-band model Hamiltonian for Bernal stacked BLG and take into account both, intrinsic symmetry breaking effects, as well as the influence of externally applied fields. Using a Hartree-Fock treatment, we study the ground state spin and isospin phases as a function of external magnetic and electric field strengths. For the different filling factors of the zero energy multiplet we predict the number of phases, as well as the nature and the properties of the respective phase transitions.

[1] Angelika Knothe and Thierry Jolicœur, arXiv:1609.04983

O 94.13 Thu 18:00 TRE Ma

Graphene-multiferroic interfaces for spintronics applications — •ᴢᴇɪʟᴀ ᴢᴀɴᴏʟʟɪ — Institute for Theoretical Solid State Physics, RWTH Aachen University and ETSF, D-52056 Aachen, Germany.

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. A very long spin diffusion length and high carrier mobility make graphene attractive for spintronics. The coupling between ferroelectricity and magnetism, which characterises magnetoelectrics, opens the way towards unique device architectures. In this work[1], we combine the features of both materials by investigating the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and $BaMnO_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones ($\sim$300 meV) is achieved. We also show how doping with acceptors can make the high-mobility region of the electronic bands experimentally accessible. This suggests a series of possible applications in spintronics (e.g. spin filters, spin injectors) for hybrid organic-multiferroic materials and reveals hybrid organic-multiferroics as a new class of materials that may exhibit exotic phenomena such as the quantum anomalous Hall effect and a Rashba spin-orbit induced topological gap.

[1] Z. Zanolli, Scientific Reports, 6, 31346 (2016)