

O 87: Graphene: Electronic Structure

Time: Thursday 15:00–18:15

Location: MA 041

O 87.1 Thu 15:00 MA 041

Tuning the electronic structure of artificial graphene with potential modulation — ●PILKWANG KIM and CHEOL-HWAN PARK — Department of Physics, Seoul National University, Seoul 151-747, Korea

Among the many different directions of research for tuning the electronic properties of massless Dirac fermions residing in materials like graphene, one of the promising candidates is the artificial graphene system where a conventional two-dimensional electron gas is modulated by external periodic potential, as first predicted theoretically [1,2]. Recently, experimentalists have confirmed the existence of massless Dirac fermions originating from metallic surface states [3,4]. In this presentation, we discuss our theoretical study on the possibility of tuning the electronic properties of massless Dirac fermions residing in 2DEG by exploiting the external potential degree of freedom. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141).

[1] C.-H. Park and S. G. Louie, *Nano Lett.* 9, 1793 (2009).

[2] M. Gibertini, A. Singha, V. Pellegrini, M. Polini, G. Vignale, A. Pinczuk, L. Pfeiffer, and K. West, *Phys. Rev. B* 79, 241406 (2009).

[3] K. K. Gomes, W. Mar, W. Ko, F. Guinea, and H. C. Manoharan, *Nature* 483, 306 (2013).

[4] S. Wang, L. Z. Tan, W. Wang, S. G. Louie, and N. Lin, *Phys. Rev. Lett.* 113, 196803 (2014).

O 87.2 Thu 15:15 MA 041

Using collective electrostatic effects to tune the electronic structure of graphene — ●GERNOT J. KRABERGER¹, DAVID A. EGGER^{1,2}, and EGBERT ZOJER¹ — ¹Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — ²Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

Graphene has unique structural and electronic properties, which have attracted huge research interest since its isolation. As a prerequisite of using this material in devices, it is necessary to modify its properties in a controlled way that it fits the needs of the application. This work uses density functional theory calculations to investigate a new approach to change the electronic structure of graphene: using the collective field of a highly ordered arrangement of dipoles to shift the potential in specific regions of graphene (i.e., exploiting so-called collective electrostatic effects). First we discuss a "proof-of-concept" model system: Along a line in graphene, pairs of neighboring carbon atoms are replaced by a boron and a nitrogen atom. Each of the resulting BN-pairs exhibits a dipole moment, which means that a one-dimensional chain of dipoles is formed. This chain impacts the electrostatic potential in its surroundings such that the electronic states in graphene are locally shifted relative to the Fermi level. With two oppositely oriented lines of dipoles it is then even possible to localize states in well-defined stripes. Finally, we explore to what extent similar effects can be generated by assembling rows of quadrupolar molecules on top of the graphene sheet instead of modifying the graphene layer itself.

O 87.3 Thu 15:30 MA 041

Graphene on weakly interacting metals: Dirac states vs. surface states — ●WOUTER JOLIE, FABIAN CRAES, and CARSTEN BUSSE — II. Physikalisches Institut, Universität zu Köln, Germany

The epitaxial growth of graphene and other two-dimensional materials on metal surfaces has become a well-established procedure and is extensively used for studies of the electronic properties of two-dimensional materials using surface science methods. However, the substrate itself can have a significant contribution to these properties. We demonstrate this on three different systems: graphene on a thick silver film on Ir(111), graphene on one monolayer of silver on Ir(111), and graphene on Ir(111). We explore the interplay between the states of the substrate (in form of nearly free surface states) and the states of the two-dimensional material on top (in form of graphenes' Dirac fermions) with scanning tunneling spectroscopy, a technique sensitive to the local density of states of the surface. We show that, when present, the surface state represents the dominant contribution in form of Friedel oscillations and confined states on graphene quantum dots. We compare these findings with a system with suppressed surface states where a clear feature of graphene is found in the density of states.

O 87.4 Thu 15:45 MA 041

Size quantization effects in quasiparticle interference on epitaxial graphene nanoflakes — ●JULIA TESCH¹, PHILIPP LEICHT¹, FELIX BLUMENSCHNEIN¹, ANDERS BERGVALL², TOMAS LÖFWANDER², LUCA GRAGNANELLO¹, and MIKHAIL FONIN¹ — ¹Universität Konstanz, Konstanz, Germany — ²Chalmers University of Technology, Göteborg, Sweden

Graphene nanostructures represent an exciting topic for research, as a strong spatial confinement together with the edge structure impose new electronic properties, making them promising candidates for future nanoscale electronic units. Here, we investigate by means of low-temperature scanning tunnelling microscopy and spectroscopy oblong quasi-freestanding epitaxial graphene nanoflakes prepared on Ag(111) and Au(111) by intercalation with virtually no edge bonding [1]. We implement quasiparticle interference (QPI) mapping to analyze standing wave patterns arising from elastic scattering processes within a single nanoflake. The Fourier analysis of the obtained QPI maps shows that in addition to ringlike structures due to the *intervalley* and *intravalley* scattering observed for large graphene sheets, additional scattering features are visible, which can be related to the transverse modes in a nanoflake [2]. Our experimental results are supported by tight-binding calculations of realistic flakes, which very well reproduce the experimentally observed fingerprints of confinement in the Fourier transform of the standing wave patterns.

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

O 87.5 Thu 16:00 MA 041

Graphene-supported metal clusters: A two photon photoemission study — KIRA JOCHMANN and ●THORSTEN BERNHARDT — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

During the last decade considerable attention was drawn to the growth of graphene on metal single crystal surfaces, where it provides an ideal template for the ordered growth of regular metal cluster arrays. Building on various investigations about the detailed growth of these cluster super-lattices, we make use of the possibility to easily grow nanostructures with equally spaced and mono-disperse clusters for fundamental research in laser selective photochemistry. Our new experimental setup enables time-resolved measurements due to a femtosecond laser system on the one hand and surface analysis via scanning tunnelling microscopy on the other hand. In first light interaction measurements time-resolved two-photon photoemission spectroscopy (2PPES) was applied to gain an insight into the unoccupied electronic structure of the Ir(111)/graphene/Ir cluster system at different graphene and cluster coverages. In subsequent experiments the combination of femtosecond laser pump-probe mass spectrometry with resonance enhanced multi-photon ionization and STM will be employed to reveal photo-dissociation dynamics of different adsorbate molecules with spatio-temporal resolution.

O 87.6 Thu 16:15 MA 041

From ribbons to constrictions: STM lithography on ballistic sidewall graphene nanoribbons — ●JENS BARINGHAUS¹, MIKKEL SETTNES², and CHRISTOPH TEGENKAMP¹ — ¹Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — ²Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

The selective graphene growth on the sidewalls of SiC mesa structures produces well-ordered graphene nanoribbons (GNR) with exceptional transport properties. Using a 4-tip STM, a probe spacing and temperature independent conductance of e^2/h is found, indicating single channel ballistic transport even at room temperature [1]. The robustness of the ballistic channel makes these GNR ideal templates for morphological alterations. For this purpose, one of the STM tips is used for local lithography. Careful control over the feedback parameters and the bias voltage allows to either fully cut the ribbon or to create narrow, a few nm wide constrictions. Every STM lithography step is monitored directly by local transport. After a full cut, the transport characteristics of the sidewall GNR are completely destroyed. In contrast, in narrow constrictions the ballistic channel is preserved, but only present at bias voltages exceeding 10 mV. Additionally, localized

currents manifest as resonances in the IV curves at bias voltages of about 8 mV. Using a standard tight binding and recursive Green's function approach, the resonances are found to be robust against temperature as well as different types of disorder, e.g. Anderson or edge disorder.

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

O 87.7 Thu 16:30 MA 041

Chiral Enhanced Phonon Spectroscopy of Graphene — ●FABIAN D. NATTERER¹, YUE ZHAO^{1,2}, JONATHAN WYRICK¹, WEN-YING RUAN³, YANG-HAO CHAN⁴, MEI-YIN CHOU^{3,4}, NIKOLAI B. ZHITENEV¹, and JOSEPH A. STROSCIO¹ — ¹Center for Nanoscale Science and Technology, NIST, Gaithersburg, USA — ²University of Maryland, College Park, USA — ³Georgia Institute of Technology, Atlanta, USA — ⁴Academia Sinica, Taipei, Taiwan

In graphene, many phenomena are driven by the interaction with phonons, such as the relaxation of hot carriers or the mediation of many-body interactions. The proper characterization of phonons can therefore shed important insights into graphene based devices. Such devices were characterized by inelastic electron tunneling spectroscopy (IETS) but weak signals and other spectral features obscured a clear distinction between phonons and miscellaneous excitations. In this talk, I show that we are able to map large parts of the graphene phonon density of states by using a back gated graphene device, where the charge carrier density can be varied in magnitude and sign. Our averaging technique combines individual IETS data, obtained over the entire charge carrier range, with the benefit of improving the signal for inelastic excitations. Surprisingly, we observe that the graphene phonon intensity is enhanced when the charge carrier type is switched, indicating that this amplification occurs whenever the inelastic transition allows a change in the graphene chirality. The chiral enhancement follows a linear trend with energy and reaches almost an order of magnitude for the highest mode.

O 87.8 Thu 16:45 MA 041

Luminescence of Graphene in the Visible Spectral Range after Short-Pulse Excitation in the Near Infrared — ●MARTIN ROTHE, GÜNTER KEWES, NIKOLAI SEVERIN, JÜRGEN P. RABE, and OLIVER BENSON — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Graphene is well known for its unique electronic and optical properties. The study and manipulation of its nonlinear optical response at energies in the range of visible light is of interest for the understanding of its charge carrier dynamics in this energy regime [1]. We find a broad luminescence of graphene and graphene multilayers in the entire visible spectral range after excitation with fs laser pulses in the near infrared. The spectrum that starts even above twice the excitation energy indicates multi-photon absorption or efficient electron scattering processes. This method of luminescence excitation is not only well suited for imaging with high contrast but can also gain insight into fundamental electron relaxation and collective excitation processes [2].

[1] Liu, et al., Phys Rev B: **82**, 081408 (2010)

[2] Lange, et al., arXiv:1404.6518 (2014)

O 87.9 Thu 17:00 MA 041

Electroluminescence from carbon-based nanostructures — ●JI HOON RYOO and CHEOL-HWAN PARK — Department of Physics, Seoul National University, Seoul 151-747, Korea

Light emission from carbon nanostructures upon current flowing reflects their novel electronic structures and is important for applications purposes. Peculiar emission versus photon energy profiles in the electroluminescence from carbon nanostructures have been attributed to inter-band electronic transitions [1], electron-phonon interactions [2] and interference effects [3]. In this presentation, we discuss the origin of multi-peak intensity versus energy feature in the electroluminescence from graphene based on recent experimental results, and look into how the electronic structure of graphene affects its electroluminescence. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141). Computational resources have been provided by Aspiring Researcher Program through Seoul National University (SNU) in 2014.

[1] D. Mann, Y. K. Kato, A. Kinkhabwala, E. Pop, J. Cao, X. Wang, L. Zhang, Q. Wang, J. Guo, H. Dai, Nature Nanotech. **2**, 33-38 (2007).

[2] S. Essig, C. W. Marquardt, A. Vijayaraghavan, M. Ganzhorn, S. Dehm, . Henrich, F. Ou, A. A. Green, C. Sciascia, F. Bonaccorso, K.-P. Bohnen, H. v. Löhneysen, M. M. Kappes, P. M. Ajayan, M. C. Hersam, A. C. Ferrari, R. Krupke, Nano Lett. **10**, 1589-1594 (2010).

[3] M. Engel, M. Steiner, A. Lombardo, A. C. Ferrari, H. v. Löhneysen, P. Avouris, R. Krupke, Nature Comm. **3**, 906 (2012).

O 87.10 Thu 17:15 MA 041

Structure and electronic states of the zig-zag graphene/h-BN interface — ●ROBERT DROST¹, ANDREAS UPPSTU², KEZILEBIEKE SHAWULIENU¹, FABIAN SCHULZ¹, SAMPASA K. HÄMÄLÄINEN¹, MIKKO ERVASTI², ARI HARJU², and PETER LILJEROTH¹ — ¹Department of Applied Physics, Aalto University School of Science, Finland — ²COMP Centre of Excellence and Helsinki Institute of Physics, Department of Applied Physics, Aalto University School of Science, Finland

Some of the most exciting properties of graphene (G) are only realised in atomically precise nanostructures. The zig-zag (ZZ) edges of this two-dimensional crystal host localised states that have been proposed to be used in spin- and valleytronic applications: Using the spin degree of freedom of the electron or the valley degree of freedom of the honeycomb crystal structure to transmit and process information. While well studied theoretically, experimental realisations remain challenging. We passivate the ZZ edge of epitaxial G with hexagonal boron-nitride (BN), a 2D insulator isostructural to G, to preserve the edge state in the band gap of the insulator. We investigate the growth of atomically perfect G/BN heterostructures on Ir(111) and Ni(111) substrates and discuss the effect of varying substrate interaction. The intrinsic properties of the G/BN interface may be revealed by intercalation with gold. Using low-temperature STM, we demonstrate the existence of a localised electronic state on the ZZ oriented G/BN interfaces. Tight binding and DFT calculations show that the interface retains many important properties of the graphene edge state.

O 87.11 Thu 17:30 MA 041

Embedding graphene quantum dots into hexagonal boron nitride — FERDINAND FARWICK ZUM HAGEN¹, CAIO SILVA¹, CHRISTOPH SCHLUETER², NICOLAE ATODIRESEI³, WOUTER JOLIE¹, DANIELA DOMBROWSKI¹, ANTONIO J. MARTINEZ-GALERA¹, DOMENIK ZIMMERMANN¹, ULRIKE SCHRÖDER¹, VASILE CACIUC³, THOMAS MICHELY¹, STEFAN BLÜGEL³, TIEN-LIN LEE², and ●CARSTEN BUSSE¹ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Diamond Light Source, Didcot, UK — ³Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Graphene (gr) nanostructures can be stabilized by embedding them into an insulating matrix. Hexagonal boron nitride (hBN) is especially suited as it is isostructural to graphene, and dangling C bonds can be satisfied by B and N. In this study, we used sequential epitaxial growth of gr and hBN on Ir(111) to embed graphene quantum dots (GQDs).

First, we investigate pristine hBN/Ir(111) with special attention to the hBN-substrate interaction which is characterized by the local varying layer height as determined with x-ray standing waves (XSW), complemented by density functional theory (DFT) calculations. Distinct differences with respect to gr/Ir(111) are found: A stronger corrugation within the moiré and an enhanced chemical interaction in the strongly bound parts of the supercell. Second, the edge atoms of GQDs on Ir(111) are investigated and an enhanced C-substrate interaction is found. Third, the chemical and structural changes at these edges upon embedding in hBN are probed. The in-plane structure is analyzed using scanning tunneling microscopy (STM).

O 87.12 Thu 17:45 MA 041

Single 3d transition metal atoms on multi-layer graphene systems: electronic configurations, bonding mechanism and role of the substrate — VIOLETTA SESSI⁶, SEBASTIAN STEPANOW^{1,2}, ALEXANDER N. RUDENKO³, SÖREN KROTZYK¹, KLAUS KERN¹, FANNY HIEBEL⁴, PIERRE MALLET⁴, JEAN-YVES VUILLEN⁴, ONDŘEJ ŠIPR⁵, ●JAN HONOLKA^{1,5}, and NICK B. BROOKES⁶ — ¹Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — ²Department of Materials, ETH Zürich, Switzerland — ³Radboud University Nijmegen, Inst. for Molecules and Materials, Netherlands — ⁴Institut Néel, CNRS-UJF, Grenoble, France — ⁵Inst. of Physics, ASCR, Prague, Czech Republic — ⁶ESRF, Grenoble, France

We present our recent study on electronic configurations of Fe, Co, Ni and Cu adatoms on graphene and graphite by x-ray magnetic circular dichroism and charge transfer multiplet theory [1]. A delicate interplay between long-range interactions and local chemical bonding is found to influence the adatom equilibrium distance and magnetic moment. The results for Fe and Co are consistent with purely physisorbed species having, however, different 3d-shell occupations on graphene and

graphite (d^{n+1} and d^n , respectively). On the other hand, for the late 3d metals Ni and Cu a trend towards chemisorption is found, which strongly quenches the magnetic moment on both substrates.

[1] V. Sessi et al., New J. of Physics 16, 062001 (2014) [Fast Track Communication]

O 87.13 Thu 18:00 MA 041

Ab initio calculation of XNLD in reflection of graphene —

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The reflection spectroscopy and in particular angular dependence of the x-ray natural linear dichroism (XNLD) were calculated on free standing monolayered graphene. The anisotropic XNLD was computed in the single electron picture within the framework of the DFT. The excitations stemming from carbon K-edge are considered. The spectral shape of the XNLD is compared with recorded data. The dependence of the reflection spectroscopy, here XNLD, based on the change of the electronic structure of bi-layer and tri-layered graphene is predicted.