

## O 39: Poster Tuesday: 2D Materials

Time: Tuesday 18:00–20:00

Location: Poster D

O 39.1 Tue 18:00 Poster D

**Electric pathways on the nanoscale** — ●JOHANNES APROJANZ<sup>1</sup>, PANTELIS BAMPOULIS<sup>2,4</sup>, ALEXEI A. ZAKHAROV<sup>3</sup>, HAROLD J. W. ZANDVLIET<sup>2</sup>, and CHRISTOPH TEGENKAMP<sup>1,4</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz, Germany — <sup>2</sup>Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — <sup>3</sup>MAX IV Laboratory and Lund University, 221 00 Lund, Sweden — <sup>4</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The electronic performance of graphene nanoribbons (GNRs) is essentially influenced by their edge termination and environment. Hence, the integration of these graphene nanostructures in future carbon-based nanoelectronics demands a profound understanding of charge transport as well as the identification of defects and interactions with the substrate, which crucially limit the propagation of charge carriers. In this study, we explore the electronic properties of both zig-zag (zz) and armchair (ac) GNR epitaxially grown on SiC templates. By means of comprehensive lateral force, conductive atomic force and nanoprobe measurements, we have directly imaged a nanoscale conductive channel, located at the bottom edge of a zz-GNR, and confirmed its ballistic nature by probe spacing dependent nanoprobe measurements. SiC substrate steps were identified as dominant charge scattering centers for this edge mode. Semi-conducting characteristics were observed for ac-GNR caused by the nano-faceting of the sidewall resulting in an array of mini-terraces. Finally, we have assigned buffer layer formation on flat SiC nanoterraces and suspended GNRs at their step edges.

O 39.2 Tue 18:00 Poster D

**Intricacies in Twisted bilayer graphene: Structural or Electronic?** — ●BIRCE SENA TÖMEKCE<sup>1</sup>, BÜSRA GAMZE ARSLAN<sup>1</sup>, OGUZHAN GÜRLÜ<sup>1,2</sup>, and DILEK YILDIZ<sup>1,2</sup> — <sup>1</sup>Istanbul Technical University, Department of Physics, 34460, Istanbul, Turkey — <sup>2</sup>Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland

Electronic and morphological properties of twisted bilayer graphene strongly depend on the rotation angle between the layers. Super periodic structures called as moire patterns are formed as a result of such rotation. However, properties of single/bilayer graphene may be modified due to unintentional doping by the substrate or due to the stress that is induced by lattice mismatch between graphene and the substrate. We prepared moire structures on highly oriented pyrolytic graphite (HOPG) by rotating the topmost graphene layer. This way we avoid the effect of the substrate on the final bilayer as the graphene is on its native surface. We studied the electronic and morphological properties of different moire patterns on graphene/HOPG system by means of scanning tunneling microscopy (STM) and spectroscopy (STS). We studied apparent corrugations of different moire patterns as a function of bias voltage in order to compare the electronic properties of moire patterns as a function of their periodicities [1]. In this work we discuss the formation mechanism of moire patterns in HOPG surfaces. We also show that moire patterns are mostly electronic if the rotation angle of the topmost graphene layer is relatively large and they are structural if the rotation angle is comparatively small. [1] D. Yildiz and O. Gürlü, Mater. Today Commun., 8 (2016), pp. 72-78

O 39.3 Tue 18:00 Poster D

**Transport Experiments Through Individual Graphene Nanoribbons** — ●NIKLAS FRIEDRICH<sup>1</sup>, JINGCHENG LI<sup>1</sup>, PEDRO BRANDIMARTE<sup>2</sup>, and NACHO PASCUAL<sup>1,3</sup> — <sup>1</sup>CIC nanoGUNE, 20018 San Sebastian-Donostia (Spain) — <sup>2</sup>Donostia International Physics Center, 20018 San Sebastian-Donostia (Spain) — <sup>3</sup>Ikerbasque, Basque Foundation for Science, 48013 Bilbao (Spain)

The bottom-up synthesis of atomically precise graphene nanoribbons (GNRs) envisions the production of model graphene structures with tuned electrical properties for electronic transport. However it is difficult to access experimentally the unperturbed bandstructure of ribbons, and furthermore, to probe their behaviour as electron transporting bands. In most scanning tunnelling spectroscopy (STS) experiments the GNRs are absorbed on a metallic substrate. This leads to a hybridization of the electronic orbitals of the GNRs with the metal and consequently a perturbation of the bandstructure.

Here we use the STM tip to contact one termination of 7-armchair

GNRs with different functionalizations and partially lift them from the surface, to bridge tip and sample in a typical transport configuration. Such, the hybridization between GNR and substrate is reduced and we probe the effect on the GNR's band structure as transport channels. We study the evolution of the bandstructure during the lifting process for varying functionalization and compare our experimental results to DFT calculations.

O 39.4 Tue 18:00 Poster D

**Chemical stability of graphene nanoribbons exposed to ambient conditions** — ●MOHAMMED S. G. MOHAMMED<sup>1,2</sup>, JAMES LAWRENCE<sup>1,2</sup>, ALEJANDRO BERDONCES LAYUNTA<sup>1,2</sup>, LUCIANO COLAZZO<sup>1,2</sup>, DIEGO PEÑA<sup>3</sup>, and DIMAS G. DE OTEYZA<sup>1,2,4</sup> — <sup>1</sup>Donostia International Physics Center (DIPC), San Sebastian, Spain — <sup>2</sup>Materials Physics Center, Centro de Física de Materiales (CSIC/UPV-EHU), San Sebastian, Spain — <sup>3</sup>Centro de Investigación en Química Biológica e Materiais Moleculares (CIQUS), Departamento de Química Orgánica, Universidade de Santiago de Compostela, Santiago de Compostela, Spain — <sup>4</sup>Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Graphene nanoribbons (GNRs) are extremely promising materials for optoelectronic applications. Key for the potential use of these functional materials synthesized under ultra-high vacuum is their stability to the environments faced during the device implementation, as well as during the ultimate device operation. In this work, starting from atomically precise chiral GNRs with well-defined semiconducting properties, we study the effect of their exposure to atmospheric conditions. STM high-resolution images and spectroscopic analysis show the severe degradation of both the bonding structure and the associated electronic properties of the ribbons. Through control experiments exposing the GNRs, still under vacuum, to low partial pressures of pure oxygen, we reveal its key role in the GNRs degradation.

O 39.5 Tue 18:00 Poster D

**Moiré structure of MoS<sub>2</sub> on Au(111): Local structural and electronic properties** — NILS KRANE, ●CHRISTIAN LOTZE, and KATHARINA J. FRANKE — Freie Universität Berlin, Berlin, Germany

Single-layer molybdenum disulfide (MoS<sub>2</sub>) has been of large interest in the latest years, due to features like a direct band gap, a strong spin-splitting of the valence band at the K-point or as a decoupling layer for molecules in an STM junction [1].

Here we grow MoS<sub>2</sub> epitaxially on a Au(111) surface and investigate its local structural and electronic properties. Using a combined STM/AFM at low temperatures we can identify the two different hollow sites in the Moiré superstructure and thus the orientations of the MoS<sub>2</sub> islands. Consequently we find a unique stacking order of MoS<sub>2</sub> with respect to the first two layers of the Au(111) surface [2].

Furthermore we get an insight into the band structure of MoS<sub>2</sub> with an STM [3] by measuring the decay length  $\kappa$  of the tunneling current, which depends on  $k_{\parallel}$ . We find a strong spatial dependence of  $\kappa$ , which we ascribe to the Moiré reconstruction of MoS<sub>2</sub> on Au(111). Additionally we find 0.4 eV above the conduction band minimum an MoS<sub>2</sub> state at the  $\Gamma$  point. We ascribe its existence to the interaction between the Au(111) substrate and the MoS<sub>2</sub>.

[1] Krane, *et al.*, ACS Nano, 2018, 12, 11, 11698-11703[2] Krane, *et al.*, Surface Science, 2018, 678, 136-142[3] Zhang, *et al.*, Nano Lett., 2015, 15, 10, 6494-6500

O 39.6 Tue 18:00 Poster D

**h-BCN Monolayers - a graphenic two-dimensional semiconductor** — ●CHRISTOPH DOBNER<sup>1</sup>, JAMES HOOPER<sup>2</sup>, SUMIT BENIWAL<sup>3</sup>, DANIEL P MILLER<sup>4</sup>, SHI CAO<sup>5</sup>, PETER A DOWBEN<sup>5</sup>, EVA ZUREK<sup>4</sup>, and AXEL ENDERS<sup>1,5</sup> — <sup>1</sup>Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth — <sup>2</sup>Dept. of Theoretical Chemistry, Jagellonian University, 30-060 Krakow, Poland — <sup>3</sup>Universität Erlangen-Nürnberg, 91058 Erlangen — <sup>4</sup>Dept. of Chemistry, Buffalo, New York 14260, USA — <sup>5</sup>Dept. of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, USA

The structural and electronic properties of a 2D graphenic but ternary monolayer containing atoms of carbon, nitrogen, and boron, h-BCN, is discussed based on results from scanning tunneling microscopy, angle-

resolved photoelectron spectroscopy and first-principles calculations. The epitaxial relationship between film and the Rh(111) substrate is manifested in a Moiré pattern in LEED and in the periodic buckling of the film on the substrate itself. The band structure and notably the band gap is consistent with that of a semiconductor and of the order of 2 - 3 eV. The valence band structure of *h*-BCN is dominated by bands formed of highly delocalized electrons, with an effective hole mass of  $-0.2m_e$ . The lowest-energy structural model obtained for a 2D structure wherein the precursor molecules do not thermally decompose during film growth reproduces key features of the band structure, most notably a direct semi-conducting band gap at the K-point. However, other potential *h*-BCN model structures that break the connectivity of the precursor molecule can be imagined and will be discussed.

O 39.7 Tue 18:00 Poster D

**Study of the morphology and the Dirac-type band structure of 2D semi-conductor superlattices with honeycomb geometry** — ●PIERRE CAPIOD, TOMAS MEERWIJK, JOEP PETERS, CHRISTIAAN POST, and DANIEL VANMAEKELBERGH — Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, Netherlands

2D systems with honeycomb geometry have attracted considerable interest in the last decade with unique electronic properties. Among them, the band structure of those type of materials exhibits a Dirac cone close the K-point. It would be of high interest to combine both Dirac-type band structure with the inherent semiconductor properties such as band gaps for electrical or optical switching.

The self-assembly of PbSe and CdSe semiconductor nanocrystal is possible via state-of-the-art chemistry techniques resulting in the square geometry or the wanted honeycomb geometry. Tight-binding calculations on the honeycomb geometry with CdSe nanocrystals have shown clear Dirac cones in the conduction bands and an opened Dirac cone in the valence band. The band structure exhibits as well non-trivial flat bands due to interactions between P-type orbitals.

The poster will show the results on the morphology and the characterization of the electronic properties obtained via Scanning Probe Microscopy (AFM & STM/STS). It will describe the steps from the synthesis, the preparation of the samples in UHV via annealing and ion bombardment to the characterization via LT-STM.

O 39.8 Tue 18:00 Poster D

**Luttinger liquid in a box: spectral signature of spin-charge separation in MoS<sub>2</sub> mirror twin boundaries** — ●PHILIPP WEISS<sup>1</sup>, WOUTER JOLIE<sup>2,3</sup>, CLIFFORD MURRAY<sup>2</sup>, JOSHUA HALL<sup>2</sup>, FABIAN PORTNER<sup>1</sup>, NICOLAE ATODIRESEI<sup>4</sup>, ARKADY KRASHENINNIKOV<sup>5,6</sup>, CARSTEN BUSSE<sup>2,3,7</sup>, HANNU-PEKKA KOMSA<sup>6</sup>, THOMAS MICHELY<sup>2</sup>, and ACHIM ROSCH<sup>1</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Cologne, Germany — <sup>2</sup>II. Physikalisches Institut, University of Cologne, Germany — <sup>3</sup>Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — <sup>4</sup>Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — <sup>5</sup>Helmholtz-Zentrum Dresden-Rossendorf, Germany — <sup>6</sup>Department of Applied Physics, Aalto University, Finland — <sup>7</sup>Department Physik, Universität Siegen, Germany

Electrons in one dimension are expected to fractionalize into spin and charge degrees of freedom. A candidate for the realization of a one-dimensional electron system are mirror twin boundaries in MoS<sub>2</sub>. Scanning tunneling spectroscopy indicates the doubling of states, well separated in energy due to the finite length of the boundaries.

To uncover the nature of these states we calculate the local density of states of interacting electrons in a box, using Tomonaga-Luttinger liquid theory. Comparison with the experimental spectra allows us to identify the doubled states as emergent spin and charge excitations.

O 39.9 Tue 18:00 Poster D

**Ab initio study of light-switchable properties of azobenzene-**

**functionalized MoS<sub>2</sub>** — ●HELENA OSTHUES and NIKOS DOLTSINIS — Institute of Solid State Theory, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The optical and electronic properties of multilayer molybdenum disulfide and other transition metal dichalcogenides (TMDCs) crucially depend on the interlayer spacing and, in general, on the surrounding dielectric medium [1]. We investigate layered two-dimensional materials which can reversibly alter their properties by exploiting the photoinduced *E-Z* isomerisation of covalently attached azobenzene chromophores.

In the present study, the stability of different functionalizations is analysed, and the photoswitching mechanism is studied using excited state ab initio molecular dynamics based on time-dependent density functional theory (TDDFT). The band structure and the absorption spectrum of the 2D structures are treated within the many-body perturbation theory in the *GW* approximation using a perturbative LDA+GdW approach [2] to take into account the variations in polarization and dielectric screening.

[1] Splendiani, A. *Nano Lett.* 2010, 10, 1271.

[2] Rohlfing, M. *Phys. Rev. B* 2010, 82, 205127.

O 39.10 Tue 18:00 Poster D

**Preparation of Graphene Bilayers on Platinum by Sequential Chemical Vapor Deposition** — JOHANNES HALLE, ●ALEXANDER MEHLER, NICOLAS NÉEL, and JÖRG KRÖGER — Institut für Physik, Technische Universität Ilmenau, Ilmenau, Germany

A cheap and flexible method is introduced that enables the epitaxial growth of bilayer graphene on Pt(111) by sequential chemical vapor deposition. Extended regions of two stacked graphene sheets are obtained by, first, the thermal decomposition of ethylene and the subsequent formation of graphene. In the second step, a sufficiently thick Pt film buries the first graphene layer and acts as a platform for the fabrication of the second graphene layer in the third step. A final annealing process then leads to the diffusion of the first graphene sheet to the surface until the bilayer stacking with the second sheet is accomplished. Scanning tunneling microscopy unravels the successful growth of bilayer graphene and elucidates the origin of moiré patterns.

O 39.11 Tue 18:00 Poster D

**Non-contact Energy Dissipation Through Charge Density Waves on 1T-TaS<sub>2</sub>** — ●DILEK YILDIZ, MARCIN KISIEL, URS GYSIN, and ERNST MEYER — University of Basel, Department of Physics, Basel, Switzerland

Small amount of energy is dissipated when bodies separated by a few nanometers gap are in relative motion. Non-contact friction can be measured by a highly sensitive cantilever oscillating like a tiny pendulum over the surface. This phenomena have been studied in many systems revealing structural and electronic phase transitions, quantum dots, and graphene devices. Understanding the origin of various dissipation mechanisms is still a wide open problem. Such frictional nature of layered systems, such as charge density wave (CDW) systems awaits to be investigated. Different phases of CDW on 1T-TaS<sub>2</sub>, a layered transition metal dichalcogenide (TMD), can be observed at different temperatures. The phase transition between nearly-commensurate and commensurate phases occurs at 180 K. We studied the origin of non-contact energy dissipation mechanisms on nearly-commensurate and commensurate CDW on 1T-TaS<sub>2</sub>. We studied the effect of Mott insulating state on dissipated power. The low temperature experimental results indicate that the main dissipation mechanism is Joule dissipation on commensurate CDW phase and fluctuation driven dissipation is the main mechanism on nearly-commensurate CDW phase. The spectroscopy performed on nearly commensurate phase of CDW indicates that the source of the fluctuating force and dissipation is the collective movement of weakly pinned charge density waves at room temperature.