

O 19: Graphene: Structural properties

Time: Monday 16:00–19:00

Location: WIL C107

O 19.1 Mon 16:00 WIL C107

Vertical height of quasi-free standing monolayer graphene on SiC(0001): an XSW study — ●J. SFORZINI¹, T. DENIG², T. L. LEE³, C. KUMPF¹, S. SUBACH¹, U. STARKE², F. C. BOCQUET¹, and F.S. TAUTZ¹ — ¹Peter Grünberg institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — ³Diamond light source Ltd, Harwell oxford, Didcot, Oxfordshire, United Kingdom

We investigated a quasi-free standing monolayer graphene sample[1] on SiC(0001) obtained by decoupling the buffer-layer from Si-terminated surface by hydrogen intercalation. We used X-ray Standing Wave technique (XSW), combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si and C) at the interface. Our analysis shows two different carbon species (C in the graphene layer and C in the SiC bulk); we find that the adsorption height of the graphene layer is slightly higher than theoretically predicted. The discrepancy, attributed to the very weak graphene-substrate intercalation, is still challenging for theory[2].

[1]Riedl, et. al., PRL, 103, 246804 (2009)

[2]Deretzis, et. al., Nanoscale, 5, 671-680 (2012)

O 19.2 Mon 16:15 WIL C107

Epitaxial graphene nanostructures on SiC — ●ALEXANDER STÖHR¹, STIVEN FORTI¹, ULRIKE WAIZMANN¹, THOMAS REINDL¹, JENS BARINGHAUS², ALEXEI ZAKHAROV³, CHRISTOPH TEGENKAMP², and ULRICH STARKE¹ — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²Institut für Festkörperphysik, Leibniz-Universität Hannover, Hannover, Germany — ³MAX IV Laboratory, Lund University, Lund, Sweden

In recent years a lot of effort was put into the realization of graphene devices, in view of their unique electronic properties and the potential application in logical circuits. However, for the use in logical electronics a band gap would be required. This can be achieved by confining the electrons into quasi-one-dimensional graphene stripes, called graphene nanoribbons. When patterning graphene, the altering of the electronic properties by the mechanical attack on the ribbon edges as well as residual resist is always an issue. For that matter we chose to structure the SiC-samples before growing graphene, using electron beam lithography and reactive ion etching. Subsequently, the graphene was grown at elevated temperatures, which also removed the residual resist. As a result one-dimensional stripes could be obtained and were decoupled from the substrate by intercalation of hydrogen. Characterization by low-energy electron microscopy and angle-resolved photoemission spectroscopy proves the development of quasi-free standing monolayer graphene ribbons.

O 19.3 Mon 16:30 WIL C107

Moiré-induced Brillouin zone backfolding of graphene phonons on Ir(111) — ●MICHAEL ENDLICH¹, ALEJANDRO MOLINA-SÁNCHEZ², HENRIQUE MIRANDA², LUDGER WIRTZ², and JÖRG KRÖGER¹ — ¹Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — ²Physics and Material Sciences Research Unit, University of Luxembourg, L-1511 Luxembourg

The moiré superstructure of graphene on Ir(111) leaves its characteristic footsteps in the phonon dispersion. Replica of the phonon dispersion branches of singly oriented graphene on Ir(111) have been determined throughout the entire surface Brillouin zone with angle-resolved inelastic electron scattering. These replica are rationalized in terms of phonon backfolding induced by the graphene moiré superlattice.

O 19.4 Mon 16:45 WIL C107

Back Focal Plane Imaging of Raman Scattering from Graphene — ●HARALD BUDE, XIAN SHI, NICOLAI HARTMANN, and ACHIM HARTSCHUH — Department Chemie und CeNS, LMU München, Germany

Raman Scattering Spectroscopy is a powerful technique for studying graphene and other sp² carbon materials [1]. We combined Raman Spectroscopy with back focal plane (BFP) imaging, a method used to visualize the angular distribution of emitted or scattered light. As an example BFP imaging allows to determine the orientation of sin-

gle dipolar emitters [2, 3]. For graphene on glass Raman BFP images mainly reflect the polarization characteristics of the different phonon modes. On thin gold films emission from graphene leads to the excitation of propagating surface plasmon polaritons.

[1] A. Ferrari, D. Basko, Nat. Nanotech 8, 235-246, 2013.

[2] M. Lieb, J. Zavislan, L. Novotny, J. Opt. Soc. Am. B 21, 1210-1215, 2004.

[3] N. Hartmann, G. Piredda, J. Berthelot, G. Colas des Francs, A. Bouhelier, A. Hartschuh, Nano Lett. 12, 177-181, 2012.

O 19.5 Mon 17:00 WIL C107

Ion Irradiation of Metal-Supported Graphene: Exploring the Role of the Substrate — ●CHARLOTTE HERBIG¹, HARRIET AHLGREN², SABINA SIMON¹, CARSTEN BUSSE¹, JANI KOTAKOSKI^{2,3}, ARKADY V. KRASHENINNIKOV^{2,4}, and THOMAS MICHELY¹ — ¹II. Phys. Inst., Universität zu Köln, Germany — ²Dept. of Phys., University of Helsinki, Finland — ³Faculty of Phys., University of Vienna, Austria — ⁴Dept. of Appl. Phys., Aalto University, Finland

Ion irradiation effects on 2D materials are an emerging subject, triggered by graphene's (Gr) potentials in applications. For supported Gr the effect of the substrate on ion beam damage and annealing is important. We investigate the behavior of high quality Gr, weakly coupled to Ir(111), to low energy noble gas ion irradiation by scanning tunneling microscopy (STM), molecular dynamics simulations, and density functional theory (DFT). For a freestanding layer, sputtered atoms leave the layer either in forward or backward direction. For metal-supported Gr, only C atoms carrying backward momentum are sputtered while atoms carrying forward momentum are trapped. As evident from STM and DFT, trapped C atoms form nm-sized Gr platelets at the interface upon annealing at 1000K, assisted by substrate defects. The incorporation into the Gr layer is suppressed due to high migration barriers, while diffusion into the Ir is energetically unfavorable. By measuring the area fraction of the platelets, we obtain the trapping yield, i.e., the number of trapped C atoms per incident ion. Interestingly, compared to the sputtering yield, the trapping yield for Gr on Ir(111) displays a distinctly different dependence on the ion beam angle of incidence.

O 19.6 Mon 17:15 WIL C107

Ab initio study of graphene on O-intercalated Ir(111) surface and its functionalization via molecular adsorption — ●VASILE CACIUC, NICOLAE ATODIRESEI, and STEFAN BLÜGEL — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

To integrate graphene in molecular electronics and spintronics devices it is crucial to understand how the strength of the graphene-metal electrode interaction can be specifically tuned. One possibility to loose or strengthen this interaction is to intercalate adatoms with different chemical reactivity between graphene and the metal surface in question. We will analyse this approach from first principles by considering the case of the O-intercalated graphene on Ir(111) [1]. Another path is to analyse how the adsorption of π -conjugated organic molecules can affect the electronic structure of a quasi-freestanding graphene layer. We investigated this issue by performing spin-polarized density functional theory (DFT) for a trioxotriangulene-derivate molecule [2] on graphene. Importantly, as already demonstrated in [3], for such systems it is mandatory to include the dispersion interaction and in our *ab initio* study these long-range van der Waals interactions were considered at a semi-empirical [4] or first-principle [5] level.

[1] E. Grånäs *et al.*, ACS Nano. **6**, 9951 (2012).[2] Y. Morita *et al.*, Nat. Mater. **10**, 946 (2011).[3] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).[4] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).[5] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

O 19.7 Mon 17:30 WIL C107

From two to three dimensions: The effect on the Coulomb interaction by increasing the dimensionality in layered materials — ●M. RÖSNER¹, E. SASIOGLU², C. FRIEDRICH², S. BLÜGEL², A.I. LICHTENSTEIN³, M.I. KATSNELSON⁴, and T.O. WEHLING¹ — ¹Institut für Theoretische Physik und Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — ²Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — ³I. Institut

für Theoretische Physik, Universität Hamburg, Hamburg, Germany — ⁴Radboud University Nijmegen, Institute for Molecules and Materials, AJ Nijmegen, The Netherlands

We study the Coulomb repulsion and the dielectric screening in mono-, bi- and tetralayer graphene as well as in graphite. We discuss the transition from 2D systems to the bulk structure in layered materials with regard to the (non) local Coulomb interactions. Therefore, we use *ab initio* constrained random phase (cRPA) calculations to get reliable data in a first step. By tailoring the resulting Coulomb interaction in classical electrostatic models afterwards, we find the following: In addition to the effective height of each layer especially the direction dependence and the non-locality of the dielectric function are the keys to understand the screening effects in these structures. Thereby, we discuss models to estimate the Coulomb interaction of the 2D systems by using exclusively the bulk data as input. We apply these rules to calculate the Coulomb interaction in graphene on iridium and find a very good agreement with *ab initio* data.

O 19.8 Mon 17:45 WIL C107

Graphene nanolithography with 2.5 nm precision: combining bottom-up and top-down techniques — ●ANTONIO J. MARTÍNEZ-GALERA^{1,2}, IVÁN BRIHUEGA^{1,3}, ÁNGEL GUTIÉRREZ-RUBIO¹, TOBIAS STAUBER^{1,3}, and JOSÉ M. GÓMEZ-RODRÍGUEZ^{1,3} — ¹Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ²Present address: II. Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln, Germany. — ³Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

The selective modification of pristine graphene represents an essential step to fully exploit its potential. The work presented here overcomes one of the remaining challenges key for the comprehensive integration of graphene in real devices: the realization of lithography below 10 nm sizes. Specifically, we have developed a perfectly reproducible nanolithographic technique for graphene that allows, by means of an STM tip, to modify with 2.5 nm accuracy the electronic properties of graphene monolayers epitaxially grown on Ir(111) surfaces. This method can be carried out also on micrometer sized regions and the structures so created are stable even at room temperature. As a result, we can strategically combine graphene regions presenting large differences in their electronic structure to design graphene nanostructures with tailored properties. Therefore, this novel nanolithography method could open the way to the design of nanometric graphene-based devices with specific functionalities. In particular, we explore here the possibility of developing a new platform for plasmonics.

O 19.9 Mon 18:00 WIL C107

Relaxation of compressive stresses in graphene through mobile nanoripples — ●PETER KLAVER, SHOEN ZHU, MARCEL SLUITER, and GUIDO JANSSEN — Delft University of Technology, Delft, Netherlands

Graphene monolayers have a far smaller thermal expansion coefficient than the Cu substrates on which they are often grown through CVD at high temperature. Once the Cu substrate and graphene monolayer are cooled down to room temperature, the Cu contracts 1.5-2.0% more than the graphene. Yet various experiments do not show graphene layers on Cu to be under significant compressive stress. We present molecular dynamics simulations that show that under compressive stress, small ripples of just a few nm wide appear that absorb the excess graphene area. These ripples are quite mobile, even at room temperature. Their movement offers a mechanism to remove the compressive stress in graphene while keeping it flat, by absorbing the ripples into larger ripples (like those that have formed around bunches of step edges) or by eliminating the ripples at the edges of graphene islands. The relaxation of stresses through the movement of nanoripples is somewhat analogous to flattening out a red carpet by gradually moving a wrinkle away to the carpet edge instead of pulling the entire carpet all at once. The ease with which stresses in graphene relax, is not directly determined by the corrugation energy.

O 19.10 Mon 18:15 WIL C107

Epitaxial graphene nanoflakes on Au(111) and Ag(111) —

●JULIA TESCH¹, PHILIPP LEICHT¹, LUKAS ZIELKE¹, RIKO MORONI¹, BERND ILLING¹, LUCA GRAGNANIELLO¹, FELIX BLUMENSCHNEIN¹, ELENA VOLOSHINA², LUKAS HAMMERSCHMIDT³, LUKAS MARSONER STEINKASSERER³, BEATE PAULUS³, YURIY DEDKOV⁴, and MIKHAIL FONIN¹ — ¹Fachbereich Physik, Universität Konstanz — ²Institut für Chemie, HU Berlin — ³Institut für Chemie und Biochemie, FU Berlin — ⁴Fritz-Haber-Institut der MPG, Berlin

In zig-zag edge terminated graphene nanoribbons or nanoflakes (GNFs), confinement of electrons is predicted to give rise to edge states with magnetic moments. However, the experimental observation of edge effects is impeded by the inevitable presence of substrates that interact with the flake edges, hence masking the GNFs' intrinsic properties. In the attempt of reducing the graphene substrate interaction, we use an entirely UHV based approach for the preparation of GNFs on Au(111) and Ag(111) surfaces allowing for flake sizes down to 10 nm. GNFs on Ir(111) are prepared by temperature programmed growth [1] and subsequently covered by deposition of several nm of Au or Ag. After post-annealing, the flakes diffuse through the Au or Ag film and form embedded or floating graphene flakes. In scanning tunnelling microscopy (STM), the edges of floating GNFs are found to be singly hydrogen terminated and entire flakes can be laterally displaced with the STM tip on both Au and Ag surfaces, suggesting a considerable reduction of graphene-substrate interactions compared to other metals. [1] Coraux et al., New J. Phys. 11, 023006 (2009)

O 19.11 Mon 18:30 WIL C107

Scattering and electronic structure in graphene nanoflakes on Au(111) — ●PHILIPP LEICHT¹, LUKAS ZIELKE¹, SAMUEL BOUVRON¹, JULIA TESCH¹, FELIX BLUMENSCHNEIN¹, LUCA GRAGNANIELLO¹, LUKAS MARSONER STEINKASSERER², BEATE PAULUS², ELENA VOLOSHINA³, YURIY DEDKOV⁴, and MIKHAIL FONIN¹ — ¹Fachbereich Physik, Universität Konstanz — ²Institut für Chemie und Biochemie, FU Berlin — ³Institut für Chemie, HU Berlin — ⁴Fritz-Haber-Institut der MPG, Berlin

Confinement of electrons in graphene quantum dots and nano ribbons with atomically well defined edges represents an exciting field of research, owing to predicted peculiar electronic and magnetic properties.

Here, we present scanning tunneling microscopy (STM) investigations of graphene nano flakes (GNFs) prepared by temperature programmed growth on Ir(111) [1] and subsequent intercalation of Au for electronic decoupling. The electronic properties of the graphene flakes are addressed by scanning tunneling spectroscopy. Within our atomically resolved constant-energy maps we can probe the electronic states of the graphene electrons exploiting the intervalley scattering. The hereby obtained dispersion relation shows a linear behavior and can be unambiguously discriminated from the parabolic dispersion relation of the Au(111) surface state electrons. The intervalley scattering of graphene electrons forms discs in the Fourier transforms of constant-energy maps, which include additional scattering features compared to monolayer graphene.

[1] Coraux, J. et al., New J. Phys. 11, 023006 (2009)

O 19.12 Mon 18:45 WIL C107

Improved effective theories for edge magnetism — ●CORNELIE KOOP and MANUEL SCHMIDT — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We consider the effective interaction between edge states in graphene nanoribbons. Low-energy edge states come along with a strongly enhanced density of states near the graphene edges, which makes electron-electron correlation important and gives rise to the so-called edge magnetism. In a pristine nanoribbon in first order, there is a direct ferromagnetic intra-edge coupling and an antiferromagnetic interaction between opposite edges. We study the coupling by means of an effective model yielding a separation between edge and bulk states. In particular we investigate the influence of the bulk states on the effective edge state theory via a second order Schrieffer-Wolff transformation. Using both numeric and analytic methods, we calculate various correlation functions. We discuss the results for the effective correlations between smooth edges as well as between the strongly localized states at rough edge structures.