O 17: Poster Monday: 2D Materials

Time: Monday 17:45–20:00 Location: Poster F

O 17.1 Mon 17:45 Poster F

Local charge transport in graphene devices mapped using Kelvin probe force microscopy — •Sayanti Samaddar[1], Kevin Janssen[1], Kai Sotthewes[2], Zhenxing Wang[3], Daniel Neumaier[3], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands — [3]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen

Graphene based field effect transistors (FETs) and diodes were investigated using KPFM in combination with transport. Imaging FETs, at different source to drain voltages, enables a mapping of local voltage drops occurring at various surface perturbations like defects, impurities, and wrinkles. In the regions between graphene wrinkles and the contacts, a strong enhancement of the potential gradients along the direction of current flow is observed. The response of these local voltage drops to a global back-gate is also investigated. In the second part, diodes comprised of titanium - titanium oxide - graphene heterostructures are studied, where gate voltages induce variations in the graphene work-function resulting in their superior asymmetry in comparison to metal-insulator-metal diodes [1]. We observe significant doping disorder ~ 50 meV on the graphene, which systematically decrease as the diode is tuned from the off state to the on state.

[1] M. Shaygan et al., Nanoscale 9, 11944 (2017)

O 17.2 Mon 17:45 Poster F

Electronic transport in Gold-contacted graphene on Germanium — •Simeon Bode[1], Anna Sinterhauf[1], Manuel Auge[2], Mindaugas Lukosius[3], Christian Wenger[3], Gunther Lippert[3], Hans Christian Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [3]IHP, 15236 Frankfurt (Oder), Germany

The successful growth of large-scale graphene on Ge/Si(001) is a large step towards the integration of graphene into silicon technologies [1]. However, since the exploration of graphene-based devices necessarily includes graphene-metal contacts, the quality of these contacts crucially limits the performance of the device. Therefore, an in-depth investigation of metal contacts on graphene on Ge/Si(001) is required. In this study, we use Kelvin probe force microscopy with an additionally applied electric field across the sample to analyze the local electrostatic potential of Gold-contacted graphene on Ge/Si(001). We find an exceptional sheet reistance for the graphene layer, whereas the electronic transport is significantly hindered close to the contacts due to the formation of a transition region. Additionally, element analysis using Rutherford backscattering reveals that the Au contact is not homogeneous; instead, an AuGe alloy forms in the contact region with a Gold Germanium ratio of approximately 50:50. This work is financially supported by the DFG through the SFB1073.

[1] Lukosius et al., ACS Appl. Mater. Interfaces 8, 33786-33793, 2016

O 17.3 Mon 17:45 Poster F

Atomistic simulations of chemical graphene exfoliation and carbon nanotube synthesis and of extended defects in bilayer graphene — •Florian Wullschläger, Robert Maidl, Konstantin Weber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Results of three recent molecular dynamics (MD) and density functional theory (DFT) studies on graphene and carbon nanotubes (CNTs) will be presented. Reductive graphite intercalation with alkali metals and subsequent dispersion in tetrahydrofuran (THF) leads to an almost complete exfoliation of graphite into graphene monolayers. The properties of the exfoliation product in liquid THF have been investigated by force-field MD simulations and first insights into role of different alkali metals in the exfoliation process will be given. Second, with force field and DFT calculations we identified the crucial reaction step in the on-surface synthesis of CNTs with controllable and defined chirality by rolling-up appropriate precursor molecules via cyclodehydrogenation reactions. Finally, by using a specifically adapted registry-dependent interlayer potential we show that the properties of dislocations in quasi-2D crystals, i.e. bilayer graphene, differ significantly from their 3D counterparts [1]. In addition to an in-depth structural characterization of 2D dislocations, first results on the dislocation structure in twisted graphene bilayers will be given.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, Nature **505** (2014) 533.

O 17.4 Mon 17:45 Poster F

Local Manipulation and Exfoliation of Graphene from an HOPG Surface using a Scanning Tunneling Microscope — •Suchetana Sarkar[1], Christoph Dobner[1], Andreas Raabgrund[2], and Axel Enders[1] — [1]Universitaet Bayreuth, Bayreuth,Deutschland — [2]Friedrich-Alexander-Universitaet Erlangen-Nürnberg, Erlangen, Deutschland

Among the several methods in which graphene can be fabricated, the manipulation of graphitic surfaces has long been of interest. Here, we demonstrate a reliable method of forming Single Layer Graphene (SLG) and Few Layer Graphene (FLG) through the local electro-exfoliation of the top layers of HOPG. Using an ambient scanning tunneling microscope (STM), we create triangular graphene flakes by scanning perpendicular to a step edge which can then be peeled back via a voltage ramp, thereby detaching it from the substrate.These triangular flakes are of interest as they behave like isolated graphene sheets and can therefore be studied to gain insights into the correlation between surface morphology and electronic properties and the possibility to tune local conductance by surface manipulation. Under certain conditions, the creation of graphene flakes near macroscopic defects and backfolding onto the HOPG terrace, led to the formation of Moiré patterns. By using 1,2,4-Trichlorobenzene to intercalate the layers of HOPG in solution, Moiré lattices as large as 200 nm were achieved. Subsequent STM studies show that these exhibit different lattice periodicites, from which we can determine precisely how the graphene layers are aligned.

O 17.5 Mon 17:45 Poster F

Transfer-Free, Highly Crystalline Graphene on Insulator for Novel Applications in Electronics — •Håkon Ivarssønn Røst[1], Justin W. Wells[1], Rajesh Kumar Chellappan[1], Anton Tadich[2], Zheshen Li[3], and Antonija Grubišić Čabo[4] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway — [2]Australian Synchrotron, 800 Blackburn Rd., Clayton, Victoria 3168, Australia — [3]Department of Physics and Astronomy, Ny Munkegade 120, 8000 Aarhus C, Denmark — [4]School of Physics & Astronomy, Monash University, Clayton, Victoria 3168, Australia

Problems associated with the preparation of high-quality and contamination-free graphene on semiconductor that does not heavily interact with its underlying substrate has so far hindered its large-scale integration in device structures. This study presents a method for growing graphene on silicon carbide (SiC) by means of various transition metal catalysts, with subsequent intercalation of silicon and oxygen under the graphene layers to form an electrically insulating dielectric layer. The interaction of thin metal films with thermally treated SiC mediates liberation of carbon, allowing the formation graphene on semiconductor at temperatures down to 600°C. Intercalation of silicon and oxygen then decouples the graphene from its substrate by forming an insulating silicon oxide layer. The result is highly crystalline top layers of free-standing graphene, where the thickness of the interfacial dielectric layer can be tuned by the amount of silicon that gets intercalated prior to the oxidation step.

O 17.6 Mon 17:45 Poster F

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •Sebastian Wille[1,2], Marvin Kammler[2], Martín L. Paleico[3], Jörg Behler[3], Alec M. Wodtke[1,2], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen,

Germany

To fully understand atom-surface interactions, the availability of an accurate full-dimensional potential energy surface (PES) is crucial. High-dimensional neural network potentials have been shown to provide very accurate PESs for a wide range of systems. We developed a neural network potential for H-atom at a graphene sheet by fitting to density functional theory data calculated on-the-fly in *ab initio* molecular dynamics simulations. Based on this potential, we studied the scattering under various incidence conditions (like angle, kinetic energy, temperature) and compared the results to experimental data.

O 17.7 Mon 17:45 Poster F

3d transition metal clusters on defected graphene — •Xin Chen, Yuhang Liu, and Biplab Sanyal — Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden

Adsorbing transition metal atoms on defected graphene is reported as one of the best routines to introduce magnetism in graphene. In this contribution, based on a first principles Born-Oppenheimer molecular dynamics simulations, we investigated the self-assembled processes of transition metal hexamers X_6 (X = Cr, Mn, Fe) on graphene with mono-/divacancy defects and discussed the fundamental electronic and magnetic properties of the resulting X_6 clusters on graphene from density functional theory. Interestingly, the ground state of Cr_6 and Fe_6 hexamers on divacancy graphene shows a quite small energy difference between in-plane and out-of-plane magnetism, and it can be easily manipulated by an external electric field, which promises applications in electric field assisted magnetic recording and quantum computing. We have also obtained insights into the switching of the easy magnetic axes, which revealed that specific d orbital symmetries of the transition metal atoms trapped in the vacancy site play a dominating role.

O 17.8 Mon 17:45 Poster F

Graphene at its Van Hove singularity and beyond — •Philipp Rosenzweig[1], Hrag Karakachian[1], Dmitry Marchenko[2], Kathrin Müller[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, 12489 Berlin, Germany

By intercalating ytterbium atoms underneath the carbon buffer layer on SiC(0001) we induce strong n-type doping in the resulting graphene monolayer. The π-band system shifts down such that the Van Hove singularity connecting $\overline{\mathrm{K}}$ and $\overline{\mathrm{K}}'$ via $\overline{\mathrm{M}}$ reaches the Fermi level E_F. The Fermi surface thus undergoes a Lifshitz transition, consisting of a single giant pocket around $\overline{\Gamma}$ as opposed to two pockets centered at $\overline{\mathrm{K}}$ and $\overline{\mathrm{K}}'$ for moderately-doped graphene systems. In addition, severe hybridization is observed between the graphene π-bands and the Yb $4f$ core levels near E_F, which might induce considerable spin-orbit splitting of graphene's Dirac cone [Marchenko et al., Nat. Commun. **3,** 1232 (2012)]. We further show that the doping level can be enhanced by potassium adsorption at cryogenic temperatures whereas sequential annealing at elevated temperatures leads to a gradual decrease in carrier density. Thus, via precise tuning of the experimental parameters, coherent control of graphene's doping level in the vicinity of its Van Hove singularity is achieved and the Lifshitz transition is observed in situ. Our studies might contribute to the experimental realization of exotic ground states in highly-doped graphene such as chiral superconductivity [Nandkishore et al., Nat. Phys. **8,** 152 (2012)].

O 17.9 Mon 17:45 Poster F

Intercalation of gold between graphene and silicon carbide studied by PEEM and XPS — •Philipp Weinert, Richard Hönig, Peter Roese, Karim Shamout, Malte Schulte, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Due to its outstanding electronic and mechanical properties graphene is highly interesting for many applications, for example as a new material in transistor applications and to build microscale structures.

In this study, the intercalation of gold between graphene and the substrate silicon carbide is investigated. Other investigations have shown, that covalent bounds between the the silicon carbide and the first carbon layer are released by intercalation, which leads to quasi free standing graphene.

To achieve the intercalation, samples have been coated with thin gold-films of different thickness. Subsequently, the samples have been annealed to cause the intercalation. In different steps of the annealing process, photoemission electron microscopy (PEEM) had been carried out for structural and X-ray photoelectron spectroscopy (XPS) for chemical investigation. Furthermore, the intercalation of silver between graphene and silicon carbide has been studied by PEEM.

O 17.10 Mon 17:45 Poster F

Influence of Li implantation on the transport properties of graphite flakes — •Johannes Küpper, José Barzola-Quiquia, Pablo Esquinazi, and Jan Meijer — Felix-Bloch-Institut für Festkörperphysik Universität Leipzig

The influence of Li implantation into mesoscopic thin graphite samples on their electrical transport properties were studied as a function of temperature and applied magnetic field. The temperature dependence of the electrical resistance before and after implantation is well described using a semiconducting contribution from the crystals and an additional metallic-like contribution due to the interfaces between them in parallel. We observe that with an increase of implantation dose the temperature dependence of the resistance gets more semiconducting, the resistivity increases an the magnetoresistance decreases. Fast fourier analysis of the Shubnikov de Haas oscillations indicates that the virgen sample is dominated by one carrier type, whereas for the implanted samples we observe the emergence of a new carrier type. Berry phase analysis of the Shubnikov de Haas oscillations indicates that our sample has 2D type charge carriers. Finally, using magnetic force microscoopy we investigate the effect of Li implantation on the creation of magnetic structures in these samples.