

O 23: Graphene: Electronic Properties and Transport (jointly with HL, MA and TT)

Time: Monday 16:00–19:00

Location: H17

O 23.1 Mon 16:00 H17

Epitaxial silicene - tunable hybridization with the substrate and weak interactions with epitaxial organic overlayers — ●RAINER FRIEDLEIN¹, ANTOINE FLEURENCE¹, FABIO BUSSOLOTTI^{1,2}, and YUKIKO YAMADA-TAKAMURA¹ — ¹School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), Nomi, Ishikawa 923-1292, Japan — ²present address: Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

The electronic and structural properties of epitaxial silicene formed on ZrB₂(0001) thin films grown on Si(111) wafers upon adsorption of either potassium atoms and anthracene molecules have been studied using photoelectron spectroscopy and electron diffraction. For pristine silicene, a particular, atomic-scale buckling leads to the opening of a direct band gap at the Γ point, while ZrB₂-related surface states are not affected. This is consistent with only a minor degree of hybridization between Si- and Zr-derived states. The electronic interactions at the interface can be tuned by electron donation from adsorbed potassium atoms, upon which hybridization is progressively switched on.

At 140 K, anthracene molecules are found to grow as epitaxial multilayers that exhibit a point-on-line commensurate relationship with silicene. The results indicate that the charge-density modulation associated with the buckling of silicene render the interactions with organic adsorbates as compared to graphene, which allows for specific epitaxial conditions. On the other hand, the results also confirm that silicene is strikingly different from other Si surfaces for which the presence of dangling bonds leads to chemisorption of organic adsorbates.

O 23.2 Mon 16:15 H17

Ab initio study of graphene nano domes on Ir(111) surface — ●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 Recently, in a combined experimental and theoretical work we have unveiled the bonding mechanism of graphene on Ir(111) surface as physisorption with a local chemical modulation [1]. In this contribution we extend our previous density functional theory (DFT) study to analyse the bonding of graphene nano domes on a clean and an oxygen pre-covered Ir(111) substrate.

As previously shown [1], the inclusion of the long-range van der Waals interactions is mandatory and in our *ab initio* study these dispersion interactions were considered at a semi-empirical [2] or first-principle [3] level, the latter as implemented in our real-space JuNoLo code [4]. In particular, the non-local correlation vdW-DF functional [3] provides an unique visual insight on the origin of a different graphene bonding on Ir(111) due to a non-local and a semi-local description of the correlation effects in DFT.

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).

[2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).

[3] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

[4] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

O 23.3 Mon 16:30 H17

Effects of strain on the excitonic Fano resonance in the optical spectrum of graphene — ●DANIELA ULLRICH^{1,2}, PATRICK HERLINGER¹, HARALD GIESSEN², JURGEN SMET¹, and MARKUS LIPPITZ^{1,2} — ¹Max Planck Institute for Solid State Research, Stuttgart — ²4th Physics Institute, University of Stuttgart

Using transmission and reflection spectroscopy we examine the optical response of graphene from the visible to the UV regime. The absorbance spectrum of free-standing graphene is dominated by an asymmetric peak in the UV at about 4.7 eV. We show that this resonance can be described by a simple Fano model which includes an excitonic state beneath the saddle point of graphene's band structure [1]. When strain is applied to a graphene sheet, the symmetry of the lattice and thus also of the band structure is broken. As predicted recently [2], this should result in a splitting of the absorbance peak in the optical spectrum as well as a strong dependence on polarization and lattice orientation. Here, we present our findings on the effects of strain on the Raman and reflectivity spectra of graphene on flexible substrates.

[1] Chae *et al.*, Nano Lett. **11**, 1379 (2011)

[2] Liang *et al.*, J. Mater. Res. **27**, 403 (2012)

O 23.4 Mon 16:45 H17

Probing Hot Electron Distributions in Graphene on Ni(111) with High Harmonic Radiation — ●CARSTEN WINTER¹, THORBEN HAARLAMMERT¹, LUCA BIGNARDI², PETRA RUDOLF², and HELMUT ZACHARIAS¹ — ¹Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — ²Zernike Institute for Advanced Materials, University of Groningen

Theoretical calculations and experimental observations of hot electron distributions in graphene show an initial ultrafast carrier relaxation accompanied by a population of optical phonons, which decay on a picosecond time scale. In this talk we present an experimental set-up suited to measure the lifetime of excited electrons and their relaxation dynamics via time-resolved 2PPE. Through frequency conversion by High Harmonic Generation coherent radiation at 39 eV photon energy is generated and subsequently used as the probe pulse in two-photon photoemission.

A graphene sheet was produced by decomposition of ethylene on a Ni(111) substrate. Hot electron distributions were generated in graphene on Ni(111) by applying 800nm pulses. The energy dependent lifetimes of these distributions have been measured. The lifetimes have been determined to 20-50 fs in the lower energy parts of the distribution ($E-E_F < 1\text{eV}$) and show a strong Ni-like behavior. In the upper energy parts lifetimes of 10-20 fs have been measured and a graphite-like behavior dominates.

O 23.5 Mon 17:00 H17

Reversible Photooxidation of Graphene — ●STEFAN BÖTTCHER, HENDRIK VITA, and KARSTEN HORN — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

Graphene oxide is often discussed in the context of a technical usage of graphene in future electronic devices. The necessity to obtain a tunable band gap in possible electronic applications makes graphene oxide a promising covalent modification of graphene. However, the homogeneous preparation of graphene oxide has so far been a challenging task, using mainly an aggressive chemical or complex physical treatment of graphene. Here we present a method to selectively produce graphene oxide from epitaxially grown graphene on transition metal surfaces such as Ir(111). Using NO₂ as an adsorbate we transform graphene into graphene oxide by irradiation with UV light at low temperatures, leading to specific signatures in the core and valence level photoemission and -absorption spectra. The graphene oxide thus prepared is stable up to room temperature, but its formation is thermally completely reversible to graphene at higher temperatures.

O 23.6 Mon 17:15 H17

Edge charge disorder in graphene — ●CORNELIE KOOP, MANUEL SCHMIDT, and CARSTEN HONERKAMP — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We study the interplay of edge roughness and electron-electron interaction in graphene nanoribbons. Our focus is the charge response of a rough edge to (possibly random) potentials induced by adatoms. While the bulk density response in graphene is rather small due to the vanishing density of states at the charge neutrality point, it turns out that edges show a strongly increased response - a fact that may be traced back to the presence of localized states at rough edges. The existence of these localized states depends on the structural properties of the edge. They are the disordered analogs to the well known edge states in clean zigzag ribbons and lead to a random sequence of peaks in the local density of states along the rough edge. As a consequence there may be strongly localized charges randomly distributed along the edge. We discuss the conditions for this effect, which we call edge charge disorder, its strength, and its consequences on the bulk electrons in a graphene nanoribbon.

O 23.7 Mon 17:30 H17

Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au — ●YAN LI¹, WEI ZHANG¹, MARKUS MORGENSTERN², and RICCARDO MAZZARELLO¹ — ¹Institute for Theoretical Solid State Physics and JARA, RWTH Aachen University, D-52074 Aachen, Germany — ²II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

We have carried out an *ab initio* study of the structural, electronic and magnetic properties of zigzag graphene nanoribbons (GNRs) on Cu(111), Ag(111) and Au(111). Both H-free and H-terminated GNRs are considered revealing that the nanoribbons invariably possess edge states when deposited on these surfaces. In spite of this, they do not exhibit magnetism at the edge, with the exception of H-terminated GNRs on Au(111), whose zero-temperature magnetic properties are comparable to those of free-standing GNRs. The absence of edge magnetism is due to the hybridization between the $2p_z$ orbitals of the carbon atoms and the d states of the metal and, for some models, to the charge transfer between the GNR and the surface, which shifts the edge state away from the Fermi level. Only in the case of H-terminated GNRs on Au(111) is the interaction between the substrate and the GNR sufficiently weak so as not to affect the magnetic properties of the edge state significantly.

O 23.8 Mon 17:45 H17

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy — ●JOOST VAN DER LIT¹, MARK BONESHANSCHER¹, MARI ILJAS², ARI HARJU², ANDREAS UPPSTU², DANIEL VANMAEKELBERGH¹, PETER LILJEROTH², and INGMAR SWART¹ — ¹Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — ²Department of Applied Physics, Aalto University, Finland

Recently, graphene nanostructures have gained a lot of interest since they introduce a bandgap in graphene, which is important for (opto-)electronics applications. Graphene nanoribbons can have a bandgap as large as 3 eV[1,2], which can be tuned by varying its width. By using a chemical bottom-up approach, we have synthesized graphene nanoribbons (GNR) on an Au(111) substrate[3]. By combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with reactive and non-reactive tips, we can relate the electronic properties of the GNRs with their atomic structure. Furthermore, we can use the STM tip to (i) deliberately create well-defined atomic scale defects and (ii) control the interaction with the substrate. Hence, we are able to directly study the robustness of the properties of the graphene nanostructures. [1] P. Ruffieux, et al., ACS Nano 6 (2012) 6930. [2] M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012) 713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

O 23.9 Mon 18:00 H17

Intact Dirac cones at broken sublattice symmetry: photoemission study of graphene on Ni and Co — ●DMITRY MARCHENKO¹, ANDREI VARYKHALOV¹, JAIME SÁNCHEZ-BARRIGA¹, MARKUS R. SCHOLZ¹, BART VERBERCK², BJÖRN TRAUZETTEL³, TIM O. WEHLING^{4,5}, CARLO CARBONE⁶, and OLIVER RADER¹ — ¹Helmholtz-Zentrum Berlin — ²Universiteit Antwerpen — ³Universität Würzburg — ⁴Universität Bremen — ⁵Bremen Center for Computational Materials Science — ⁶Consiglio Nazionale delle Ricerche Trieste

A band gap at the Dirac point of graphene can be created by breaking of the sublattice symmetry through epitaxial growth on a substrate crystal. One of the strongest sublattice-symmetry-breaking interactions with predicted and measured band gaps ranging from 400 meV to more than 3 eV has been attributed to the interfaces of graphene with Ni and Co, which are also promising spin filter interfaces. We apply angle-resolved photoemission to epitaxial graphene on Ni(111) and Co(0001) to show the presence of intact Dirac cones in a strongly n-doped system. Our results challenge the common belief that breaking of sublattice symmetry by a substrate and opening of the band gap at the Dirac energy are in a straightforward relation. A simple effective model of a biased bilayer structure composed of graphene and a sublattice symmetry broken layer, corroborated by density functional theory calculations, demonstrates the general validity of our conclusions.

O 23.10 Mon 18:15 H17

sp² carbon hybrid junctions — PABLO ROBERT^{1,2}, RENJUN DU¹, FAN WU¹, KRISTINA HÖNES¹, JENS MOHRMANN¹, FRANK HENNRICH¹, MANFRED KAPPES^{1,3,4}, HILBERT VON LÖHNEYSEN^{1,2,4,5}, and ●ROMAIN DANNEAU^{1,2} — ¹Institute of Nanotechnology, Karlsruhe

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Lowering the contact resistance is a key issue to improve graphene field effect device performance. The connection between a metal and graphene depends on many parameters such as the work function mismatch between the two connected material, the adsorption of the metal on graphene, the quality of the deposited material as well as the strain induced on the graphene sheet. We have studied electronic transport through carbon nanotube (CNT)-graphene and graphene-graphene junctions produced by nano-manipulation and transfer. For the CNT-graphene junctions, we first demonstrate that the influence of the CNT on the charge distribution of the graphene sheet is limited to few nanometers. Our experiments show that the junction transparency is strongly gate dependent due to the variation of the CNT-graphene distance, and the charge carrier injection occurs via a single point. For the graphene-graphene junctions, our measurements show low resistance and prove that graphene makes a good connection to graphene.

O 23.11 Mon 18:30 H17

Graphene on boron nitride microwave transistors driven by graphene nanoribbon back-gates — CHRISTIAN BENZ^{1,2}, ●MAXIMILIAN THÜRMER¹, FAN WU¹, ZEINEB BEN AZIZA¹, JENS MOHRMANN¹, HILBERT VON LÖHNEYSEN^{1,2,3,4}, KENJI WATANABE⁵, TAKASHI TANIGUCHI⁵, and ROMAIN DANNEAU^{1,2} — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — ²Institute of Physics, Karlsruhe Institute of Technology, Germany — ³DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — ⁴Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — ⁵Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan

We have designed ultra-thin graphene microwave transistors by using pre-patterned metal or graphene nanoribbon back-gates and hexagonal boron nitride (h-BN) as a dielectric substrate. Despite the inhomogeneities induced by the graphene transfer process, we show that it is possible to operate these types of devices across a broad range of microwave frequencies. For the graphene nanoribbon gates, we observe a deviation of the current gain from the usual $1/f$ trend that can be attributed to the large gate resistance of these systems as we demonstrate with our small-signal model. The scattering parameter analysis shows a very limited back-action from the channel onto the graphene nanoribbon gates. Our work thus proves that graphene microwave transistors could be driven by graphene nanoribbon gates.

O 23.12 Mon 18:45 H17

Strong gate hysteresis in graphene on mica field effect devices — ●JENS MOHRMANN¹, KENJI WATANABE², TAKASHI TANIGUCHI², and ROMAIN DANNEAU^{1,3} — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — ²Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan — ³Institute of Physics, Karlsruhe Institute of Technology, Germany

One of the outstanding properties of graphene is the unbeatable ratio of surface to volume. As a membrane of only one atomic layer of carbon, graphene is extremely sensitive to external influences. The large area contact with the substrate thus causes a large influence of the used substrate on the electronic properties of graphene. Therefore, a lot of effort is being made in order to understand the interaction between graphene and its substrate, and to find new and possibly better materials. One material under investigation is muscovite mica. The layered structure allows perfect basal (001) cleavage with atomically flat terraces, and using mechanical exfoliation, very thin crystals can be created and used as a substrate and gate dielectric. Transport measurements of graphene on mica show a very high hysteresis with respect to the gate voltage. Here, we investigate this effect using dual gated devices, with both mica and hexagonal boron-nitride dielectrics.