Epitaxial silicene - tunable hybridization with the substrate and weak interactions with epitaxial organic overlayers —

Rainer Friedlein, Antoine Fleurence, Fabio Bussolotti, and Yukiko Yamada-Takamura

The electronic and structural properties of epitaxial silicene formed on ZrB$_2$(001) 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 $\Gamma$ point, while ZrB$_2$-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.

Ab initio study of graphene nano diamonds on Ir(111) surface —

Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel

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 diamonds 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 non-loci description of the correlation effects in DFT.

Effects of strain on the excitonic Fano resonance in the optical spectrum of graphene —

Daniela Ulrlisch, Patrick Herlinger, Harald Giessen, Jürgen Smet, and Markus Lippitz

Transmission and reflectivity measurements reveal the occurrence and the central energy position of the excitonic Fano resonance in graphene. These measurements are consistent with a recent theoretical study of the Fano resonance in graphene nanoribbons [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.

Probing Hot Electron Distributions in Graphene on Ni(111) with High Harmonic Radiation —

Carsten Winter, Thorsten Haarlammert, Luca Bignardi, Petra Rudolf, and Helmut Zacharias

Theoretical calculations and experimental observations of hot electron distributions in graphene show an initial ultrafast carrier relaxation accompanied by a population of optical phonons. In this talk, we present an experimental setup to perform a femtosecond time-resolved 2PPE measurement. The graphene nanoribbon is thus prepared 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 eV) and show a strong Ni-like behavior. In the upper energy parts lifetimes of 10-20 fs have been measured and a graphene-like behavior dominates.

Reversible Photooxidation of Graphene —

Stepan Bottcher, Hendrik Vita, and Karsten Horn

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 NO$_2$ 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.

Edge charge disorder in graphene —

Cornelie Koop, Manuel Schmidt, and Carsten Honerkamp

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.

Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au —

Yan Li, Wei Zhang, Markus Morgenstern, and Riccardo Mazzerello

Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au.
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 two pz 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.

**H. 24.8 Mon 17:45 H17**

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy — *Joost van der Litt*, Mark Boneschanscher, Mari Ilijaš, Ari Harju, Andreas Uppström, Daniel Vannaekelberg, Peter Liljeros, and Ingar Swart

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 (GNRs) 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) 6030. [2] M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012) 713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

**H. 24.9 Mon 18:00 H17**

**Intact Dirac cones at broken sublattice symmetry: photoemission study of graphene on Ni and Co** — *Dmitry Marchenko*, Andrei Varykhalov, Jaime Sánchez-Barriga, Markus R. Scholz, Bart Verberck, Böörn Trauzettel, Tim O. Wehling, Carlo Carboni, and Oliver Rader

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 0.03 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(001) 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.

**H. 24.10 Mon 18:15 H17**

**sp² carbon hybrid junctions** — *Pablo Robert*, Renjun Du, Fan Wu, Kristina Hönes, Jens Mohrmani, Frank Henrich, Manfred Kappes, Hilbert von Löhniesens, and Romain Danneau

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy — *Joost van der Litt*, Mark Boneschanscher, Mari Ilijaš, Ari Harju, Andreas Uppström, Daniel Vannaekelberg, Peter Liljeros, and Ingar Swart

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 (GNRs) 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) 6030. [2] M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012) 713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

**H. 24.11 Mon 18:30 H17**

**Graphene on boron nitride microwave transistors driven by graphene nanoribbon back-gates** — *Christian Benz*, Maximilian Thümmer, Fan Wu, Ziren Ben Azziz, Jens Mohrmani, Hilbert von Löhniesens, Kenji Watanabe, Takashi Taniguchi, and Romain Danneau

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.

**H. 24.12 Mon 18:45 H17**

**Strong gate hysteresis in graphene on mica field effect devices** — *Jens Mohrmani*, Kenji Watanabe, Takashi Taniguchi, and Romain Danneau

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.