

O 45: Graphene: Adsorption, Intercalation and Doping

Time: Tuesday 18:15–20:30

Location: Poster E

O 45.1 Tue 18:15 Poster E

Intercalation of epitaxial graphene on SiC by antimony — ●SUSANNE WOLFF¹, SARAH ROSCHER¹, MARTINA WANKE¹, FLORIAN SPECK¹, CHRISTIAN RAIDEL¹, MARCUS DANIEL², FELIX TIMMERMANN³, and THOMAS SEYLLER¹ — ¹TU Chemnitz, Institut für Physik, Technische Physik, Germany — ²TU Chemnitz, Institut für Physik, Oberflächen- und Grenzflächenphysik, Germany — ³Universität Augsburg, Institut für Physik, Experimentalphysik IV, Germany

Graphene on SiC is grown epitaxially by sublimation growth. The first carbon layer grown is still covalently bound to the Si atoms of the substrate and therefore electronically inactive. Intercalation of epitaxial graphene on SiC decouples the buffer layer from the SiC substrate making it electronically active. In addition, intercalation can manipulate the structural and electronic properties. Thereby graphene can be adjusted for device applications.

In our x-ray photoelectron spectroscopy studies we investigated the intercalation of antimony on epitaxial graphene on SiC(0001). Antimony was evaporated from a Knudsen cell by molecular beam epitaxy at the surface and subsequently annealed with in a temperature range of 400°C to 500°C. Antimony shows different behavior for intercalation in ultra-high vacuum and argon atmosphere.

O 45.2 Tue 18:15 Poster E

Interaction of 10 nm-sized Co, Pd, and Ti islands with epitaxial graphene — ●ANASTASIA SOKOLOVA, FRANZISKA KILCHERT, and M.ALEXANDER SCHNEIDER — Solid State Physics, Friedrich-Alexander University Erlangen-Nürnberg, Germany

We investigated the adsorption and intercalation properties of metals (Co, Pd and Ti) relevant for contact formation on epitaxial graphene on 6H-SiC(0001) by Scanning Tunneling Microscopy (STM).

When evaporated at substrate temperatures below 100°C, all three metals form (111) and (0001) oriented ad-islands. Only titanium showed a tendency to decorate substrate step edges. Judging from the cobalt and palladium ad-island stability with respect to material pick up by the STM tip, palladium forms weaker bonds to graphene than cobalt. Titanium ad-islands could also be removed by the STM tip. However we observe in the majority of cases that the graphene underneath is removed. We take this as an indication of a strong chemical interaction between titanium and graphene.

After annealing to approximately 600°C Co and Pd readily intercalate while Ti does not. Co intercalates by forming metal islands below the graphene sheet similar in size as the previous ad-islands, while Pd additionally formed large (> 50 nm in lateral size) patches growing from step edges or holes in the graphene sheet indicating coalescence of intercalated material.

O 45.3 Tue 18:15 Poster E

Crystalline Xe underneath a monolayer of hexagonal boron nitride — ●PHILIPP VALERIUS¹, CHARLOTTE HERBIG¹, MOHAMMAD ALIF ARMAN², JAN KNUDSEN^{2,3}, and THOMAS MICHELY¹ — ¹II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany — ²Division of Synchrotron Radiation Research, Lund University, Box 118, 22100 Lund, Sweden — ³MAX IV Laboratory, Lund University, Box 118, 22100 Lund, Sweden

Exposing a monolayer of hexagonal boron nitride on Ir(111) at room temperature to Xe irradiation in the energy range from a few 100 eV to a few 1000 eV causes amorphization of the 2D layer material, as shown by low energy electron diffraction. Surprisingly, upon annealing the hexagonal boron nitride recovers to perfection, except of vacancy islands resulting from sputtering and blisters formed due to aggregation of implanted species. With scanning tunneling microscopy we image through the hexagonal boron nitride blister lid and find a superstructure corresponding in lattice parameter to what we expect for a crystalline Xe layer. X-ray photoelectron spectroscopy experiments confirm this interpretation. We conclude that due to the strong adhesion of hexagonal boron nitride to Ir(111) the pressure inside the blisters is in the GPa range. An additional peculiar feature of our experiments are noble gas filled hexagonal boron nitride blisters, which are surrounded only by bare Ir(111).

O 45.4 Tue 18:15 Poster E

Band gap engineering by Bi intercalation of graphene on Ir(111) — ●JONAS WARMUTH¹, MATTEO MICHARDI², ALBERT BRUIX FUSTÉ², TORBEN HÄNKE¹, MARCO BIANCHI², JENS WIEBE¹, ROLAND WIESENDANGER¹, BJØRK HAMMER², PHILIP HOFMANN², and ALEXANDER AKO KHAJETOORIAN^{3,2} — ¹Dept. of Physics, Hamburg University, Hamburg, Germany — ²Interdisciplinary Nanoscience Center and Department of Physics and Astronomy, Aarhus University, Denmark — ³Institute of Molecules and Materials, Radboud University, Nijmegen, Netherlands

We report on the structural and electronic properties of a single bismuth layer intercalated underneath a graphene layer grown on an Ir(111) single crystal. Scanning tunneling microscopy (STM) reveals a hexagonal surface structure and a dislocation network upon Bi intercalation, which we attribute to a $\sqrt{3} \times \sqrt{3}R30^\circ$ Bi reconstruction on the underlying Ir(111) surface. Ab-initio calculations show that this Bi reconstruction is the most energetically favorable, and also illustrate that STM measurements are most sensitive to C atoms in close proximity to intercalated Bi atoms. Additionally, Bi intercalation induces a band gap ($E_g = 0.42\text{eV}$) at the Dirac point of graphene and an overall n-doping (0.39eV), as seen in angular-resolved photoemission spectroscopy. We attribute the emergence of the band gap to the dislocation network which forms favorably along certain parts of the moiré structure induced by the graphene/Ir(111) interface.

O 45.5 Tue 18:15 Poster E

Superstructures and Phonons of Graphene on Ir(111) Induced by Li Intercalation — ●JOHANNES HALLE, NICOLAS NÉEL, and JÖRG KRÖGER — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Lithium-intercalated graphene on Ir(111) exhibits various superstructures with increasing coverages as unveiled with low-temperature scanning tunnelling microscopy. At low coverages Li always resides at one specific high-symmetry site of the moiré pattern. Compact, elongated and trefoil-like Li clusters become the building blocks of superstructures at higher coverages. Their shapes and orientations reflect local strain variations in the graphene sheet and the energy landscape of different sites in the moiré unit cell. Intercalation of Li enables the observation of graphene phonons in inelastic electron tunnelling spectroscopy. While for pristine graphene phonon features stay below the detection limit, clear signatures of M point acoustic and optical phonons appear in the spectra of Li-intercalated graphene.

Funding by the Deutsche Forschungsgemeinschaft through KR 2912/10-1 is acknowledged.

O 45.6 Tue 18:15 Poster E

Near-Saturated Hydrogenation of Graphene on Ir(111) — ●CLIFFORD MURRAY, ULRIKE SCHRÖDER, ANTONIO MARTÍNEZ-GALERA, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany

Hydrogen adsorption structures on graphene on Ir(111) have previously demonstrated their potential to modify the electronic properties of graphene (Gr) [1,2]. We have combined temperature programmed desorption (TPD) and scanning tunneling microscopy to further the understanding of this hydrogenation when close to saturation. We investigate dosage dependence of deuterium radical adsorption, diffusion thereof, and calculate coverages by calibrating TPD spectra. These spectra show two broad desorption peaks - at roughly 380K and 730K - representing two different adsorption states for deuterium on graphene. By growth of a Pt cluster superlattice we selectively block a specific area in the Gr moiré from adsorption. Subsequent radical exposure and the attenuation of the high temperature peak in desorption from this sample allows us to pin-point the binding area of the radicals. It is consistent with the formation of graphene-like patches in the moiré unit cell. We will speculate on the nature of the low temperature desorption peak.

[1] R. Balog et al., Nature Mater, 9, 315 (2010)

[2] R. Balog et al., ACS Nano, 7, 3823 (2013)

O 45.7 Tue 18:15 Poster E

Adsorption of molecules on graphene-supported iridium clusters — ●ANDREAS STOLL, KIRA JOCHMANN, and THORSTEN BERNHARDT — Universität Ulm

The adsorption of organosulfur and porphyrin molecules onto numerous metal and semiconductor substrates results in the formation of dense highly oriented self-assembled monolayer structures. Hitherto, the majority of studies dealt with the adsorption of these molecules on the Au(111) surface or on gold clusters in solution. In this contribution we investigate the adsorption of various organosulfur and porphyrin molecules on iridium clusters that were prepared on the moiré-type superstructure of graphene on Ir(111) by a combination of two photon photoemission spectroscopy and scanning tunneling microscopy (STM). The selection of this system was guided by the prospect to directly map the single chemisorbed molecules via room temperature STM. All molecules were found to exhibit unique geometric adsorption patterns on the bare Ir(111) surface, on graphene, and on the Ir clusters on graphene, respectively.

O 45.8 Tue 18:15 Poster E

Square ice sandwiched in graphene: a theoretical NMR study — ●ACHRAF JAADOUNI, EVA RAULS, WOLF GERO SCHMIDT, and UWE GERSTMANN — Uni Paderborn, Theoretische Physik, Pohlweg 55, 33100 Paderborn

Bulk water can exist in many forms, liquid, vapour and at least 16 crystalline phases, including the famous hexagonal ice [1]. Theory suggests, that many further phases can occur, if water is adsorbed on surfaces or confined in nanoscopic pores. A determination of the microscopic structure, however, provides a major challenge for experiment. Recently, locked between two graphene sheets, a new high-density phase has been observed by transmission electron microscopy (TEM) [2]. The so-called 'square ice' provides a symmetry qualitatively different from both hexagonal ice as well as graphene.

Modelling bilayer and trilayer lattices within density functional theory (DFT), we show that the phase transition from hexagonal to square ice is accompanied by a characteristic change of the NMR chemical shifts for the included protons. Hence, the detection via NMR spectroscopy appears as a promising alternative to electron imaging, in particular in case of nanostructures with a high amount of disorder, e.g. hydrophobic nanocapillaries.

[1] G. Malenkov, J. Phys. Condens. Matter 21, 283101 (2009).

[2] G. Algara-Siller et al., Nature 519, 443 (2015).

O 45.9 Tue 18:15 Poster E

Long range structure of oxygen and hydrogen adsorbed graphene — ●JAN GESENHUES and MICHAEL ROHLFING — WWU Münster

Adsorption of atomic oxygen and hydrogen on planar graphene is theoretically studied within a DFT-LDA framework. Changes in the spatial as well as electronic structure are studied in comparison to pristine

graphene. In particular large supercells are considered to determine the long range effects of the respective adsorption. Our results show that the atomic adsorption mediates geometric changes as far as 20 Å while electronic changes can be observed approximately within 15 Å.

O 45.10 Tue 18:15 Poster E

Trends in chemical reactivity of carbon allotropes — ●SEBASTIAN GSÄNGER and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The specific geometry of fullerenes, carbon nanotubes with different chirality and graphene imposes certain restrictions on the network of distributed π -bonds and therefore on their electronic properties and their reactivity towards adsorption. Using density-functional theory calculations, the adsorption energies of various adsorbates on the different allotropes was evaluated. For hydroxyl groups, adsorption patterns were analyzed and correlated with the electronic structure of the carbon allotrope. Finally, differences and similarities between the allotropes were identified and analyzed.

O 45.11 Tue 18:15 Poster E

Higher Order Corrected Spectroscopy at the Carbon K Edge — ●CHRISTINE JANSING¹, HANS-CHRISTOPH MERTINS¹, ANDREAS GAUPP^{1,2}, ANDREY SOKOLOV², MARKUS GILBERT¹, ANDREAS SCHÜMMER¹, HUD WAHAB³, HEIKO TIMMERS³, and SUK-HO CHOI⁴ — ¹Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — ²HZB, Albert Einstein Str. 15, D-12489 Berlin — ³University of New South Wales, Canberra, ACT 2600, Australia — ⁴Kyung Hee University, Yongin 446-701, Korea

We present the experimental determination of disturbing higher order synchrotron radiation across the carbon K edge at a soft x-ray beamline and a procedure to correct spectra of carbonaceous materials like highly oriented pyrolytic graphite (HOPG) or graphene. Measurements in the soft x-ray regime suffer from an enormous loss of photon flux at the C K edge, caused by carbon contamination of the beamlines optical elements. The unavoidable contaminations result from residual organic molecules in the beamline getting cracked by synchrotron radiation and absorbed as adventitious carbon on mirrors. In particular first order radiation is absorbed so that incident light has large contributions from higher order wavelengths. We determined the amount of higher order light of up to 60% in the π^* -resonance of carbon exploiting a second monochromator and alternatively using a simple filter. We show that both methods reveal a reliable set of data to correct on higher order distortion of our experimental reflection and absorption spectra. This correction procedure can be applied to any carbonaceous material's spectra.