Time: Wednesday 10:30–13:00

Location: MA 041

O 41.1 Wed 10:30 MA 041

Morphology dependent kinetics of oxygen intercalation into graphene/Ir(111) — \bullet ULRIKE SCHRÖDER¹, ELIN GRÅNÄS², TIMM GERBER¹, JAN KNUDSEN², MOHAMMAD ARMAN², KARINA SCHULTE³, JESPER ANDERSEN², and THOMAS MICHELY¹ — ¹II. Phys. Institut, Universität zu Köln — ²Division of Synchrotron Radiation Research, Lund University — ³MAX-Lab, Lund University

Stability of graphene in the presence of gases and at elevated temperatures is of crucial importance for various applications, including its use as a template for well-ordered cluster growth [1].

We investigate the morphology and temperature dependence of oxygen intercalation into graphene/Ir(111) by STM measurements, complementary to our XPS results. A full monolayer of graphene grown with the TPG+CVD method [2] is remarkably stable against O_2 exposure. No intercalation takes place and etching of graphene is only observed at temperatures above 700 K. In STM the onset of etching is visible by hexagonal etch holes in the graphene after O₂ exposure at 740 K. In contrast, O intercalates readily at 400 K under large graphene flakes that cover only 50% of the surface. Surprisingly, smaller flakes resist intercalation at 400 K. Details of the intercalation kinetics can be distinguished by analyzing differences in moiré contrast and apparent graphene heights that are due to oxygen intercalation. Decoupling of graphene from the metal substrate is directly investigated through the effect intercalation has on the formation of metal cluster lattices. [1] N'Diaye et al.; NJP 2009, 11, 103045. [2] van Gastel et al.; APL 2009, 95, 121901.

O 41.2 Wed 10:45 MA 041

Intercalation of O_2 and CO on graphene grown on Ir(111) — •ELIN GRÅNÄS¹, JAN KNUDSEN¹, TIMM GERBER², ULRIKE SCHRÖDER², MOHAMMAD ARMAN¹, KARINA SCHULTE³, THOMAS MICHELY², and JESPER ANDERSEN¹ — ¹Division of Synchrotron Radiation Research, Lund University, Sweden — ²II. Physikalisches Institut, Universität zu Köln, Germany — ³MAX IV Laboratory, Lund University, Sweden

Graphene is a potential support material for catalytic model systems since it is chemically inert at room temperature and has a high thermal stability in ultra-high vacuum (UHV). The stability in a controlled gas environment at slightly elevated temperatures (300 - 500 K), typical for many catalytic processes, is however virtually unexplored. In this contribution we will discuss the stability of graphene supported on Ir(111) in common gases such as O_2 and CO in the pressure interval from 10^{-8} to 0.1 mbar.

We find that both CO and O₂ intercalate when holes are present in the graphene film, and with the use of X-ray photoemission spectroscopy movies we follow the intercalation process in real time. Surprisingly our studies reveal that intercalation of O₂ and CO starts already close to room temperature. One important consequence of this is that graphene grown on transition metals often is converted to graphene floating on a layer of adsorbates when it is exposed to either O₂ or CO at slightly elevated temperatures. Finally we will discuss scanning tunneling microscopy studies of the partly intercalated films, that reveal how the intercalation proceeds.

O 41.3 Wed 11:00 MA 041

Intercalation of transition metals underneath graphene on Rh(111) and $Ir(111) - \bullet MIKHAIL FONIN^1$, PHILIPP LEICHT¹, KON-STANTIN KRAUSERT¹, LUKAS ZIELKE¹, MURIEL SICOT¹, and YURIY DEDKOV² - ¹Fachbereich Physik, Universität Konstanz, Konstanz, Germany - ²SPECS Surface Nano Analysis GmbH, Berlin, Germany Structure and electronic properties of atomically sharp interfaces between graphene and transition metal surfaces are both of fundamental and technological interest in view of possible device applications. Intercalation of other metals between graphene and metallic substrate can be used to controllably modify the electronic properties of the graphene/metal interfaces.

In this work we report on the intercalation of transition metals (Fe, Co, Ni, Au) underneath a graphene monolayer on Rh(111) and Ir(111). Scanning tunneling microscopy (STM) and photoemission spectroscopy (PES) are implemented to study the atomic structure as well as the electronic properties of the intercalation systems. We show that intercalation starts already at temperatures as low as 400° C and

can be efficiently performed up to 600° C without any visible damage of the graphene overlayer. Atomically-resolved imaging of the graphene surface after intercalation shows considerable changes of the moire structure on top of intercalated metal patches due to the changing of the bonding strength. The corresponding changes in the electronic structure of graphene are reflected in the PES spectra.

O 41.4 Wed 11:15 MA 041 Induced magnetism in transition metal intercalated graphitic systems — •MOUSUMI UPADHYAY KAHALY, THANESHWOR KALONI, and UDO SCHWINGENSCHLÖGL — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

Inducing spin-polarization in graphene by doping transition metal (TM) atoms is interesting because it can modify the electronic states locally. Precise knowledge of the TM-C interaction is important for understanding carbon nanotube growth, fuel cells, and the role of implanted magnetic atoms, such as Fe, for the magnetic order. For these reasons, we will discuss first-principles results on the structure, chemical bonding, electronic properties, and the spin-polarization induced by Mn, Fe, Co, Ni, and Cu atoms intercalated between adjacent C layers in a three-dimensional graphitic network in aba and aaa stacking. Our results point to a strong preferential bonding of the transition metal atoms in specific lattice sites. The moment induced by Mn, Fe, and Co turns out to vary from 1.38 μ_B to 4.10 μ_B , whereas intercalation of Ni and Cu does not lead to a magnetic state. Overcoming the fundamental problem of the high mobility of transition metal atoms in graphene, this preferential bonding and the selective induction of spin-polarization opens up a way to graphitic Kondo systems. Intercalated graphitic materials are likely to provide new possibilities for applications in spintronics and nanoelectronics.

O 41.5 Wed 11:30 MA 041

Intercalation of Ni underneath graphene on Ir(111) — •PHILIPP LEICHT, KONSTANTIN KRAUSERT, LUKAS ZIELKE, and MIKHAIL FONIN — Fachbereich Physik, Universität Konstanz, Germany

Interfaces of ferromagnetic materials and graphene have been reported as candidates with potential spin filtering capabilities [1]. Apart from direct growth of graphene on ferromagnetic Ni substrates, ferromagnetic metals can be intercalated between graphene and the substrate interface for many graphene/metal systems [2]. Thereby pre-deposited metals can penetrate graphene upon thermal annealing at moderate temperatures.

In this work we present the investigation of Ni intercalation underneath a graphene monolayer on Ir(111). We use scanning tunneling microscopy (STM) to determine the structure of the prepared samples with the intercalated Ni amount ranging from a submonolayer to few monolayers. Intercalation preferentially occurs at step edges forming areas with strongly increased moiré corrugation and decreased average distance of graphene from the intercalant compared to graphene/Ir(111). The stronger corrugation in conjunction with a shift of the C 1s core level observed in x-ray photo-electron spectroscopy suggests a strong bonding between graphene and Ni.

 Karpan, V. M. et al. Phys. Rev. B 78, 195419 (2008) [2] Huang, Li et al. Appl. Phys. Lett. 99, 163107 (2011)

O 41.6 Wed 11:45 MA 041

Spin-polarized STM of cobalt intercalated graphene/Ir(111) — ●RÉGIS DECKER¹, JENS BREDE¹, NICOLAE ATODIRESEI², VASILE CACIUC², STEFAN BLÜGEL², and ROLAND WIESENDANGER¹ — ¹Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg — ²Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich

It has been shown that graphite intercalation compounds present peculiar characteristics such as dramatic changes in the transport, optical and catalytic properties compared to bulk graphite, or even superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. In particular, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, using the spin-polarized STM technique, we are able to study the structure, as well as the local electronic and magnetic properties of graphene on a magnetic substrate, where the magnetic substrate is obtained by the intercalation of a cobalt layer between graphene and an Ir(111) surface. The experimental results are compared to DFT calculations.

O 41.7 Wed 12:00 MA 041

Structural and electronic properties of the graphene/Al/ Ni(111) intercalation system — •ELENA VOLOSHINA¹, MAR-TIN WESER², STEFAN BÖTTCHER², KARSTEN HORN², and YURIY DEDKOV^{2,3,4} — ¹Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ³Institut für Festkörperphysik, Technische Universität Dresden, Germany — 4 SPECS Surface Nano Analvsis GmbH, Germany

The atomic and electronic structure of the graphene/Al/Ni(111) system is studied via combination of experimental methods and density functional theory calculations. It has been demonstrated, that the graphene layer can be effectively decoupled from the ferromagnetic substrate via intercalation of the sp metal [1]. Despite the symmetry in the graphene lattice is broken in the trilayer under consideration, there is no sizable energy gap for the π states around the K point of Brillouin zone. In this talk, properties of graphene/Ni(111) and graphene/Al/Ni(111) are compared. The perspectives of application of the Al-based intercalation-like systems are discussed.

[1] E. N. Voloshina, A. Generalov, M. Weser, S. Boettcher, K. Horn, Yu. S. Dedkov, arXiv:1108.3002 (2011); New. J. Phys. (accepted).

O 41.8 Wed 12:15 MA 041

- •Jörg Doppler, Florian Mittendorfer, and Josef Redinger Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria

ARPES Data $\operatorname{graphene}/\operatorname{Re}$ from experiments on and graphene/Ag/Re(0001), which features an additional intercalated Ag monolayer, demonstrate that the strong interaction of Gr/Re is significantly lowered as soon as Ag is introduced. It is also found that the Ag atoms grow epitactically, and we have evidence of a hybridization of the Ag bands with graphene's π -state. We study the electronic structure of Gr/Ag(111)/Re(0001) by means of numerical ab-initio DFT calculations employing the program VASP. The properties of gr/Ag/Re were determined in a simplified approach by examining a (1x1) cell for the two equilibrium lattice constants of Re and Gr, i.e. either stretching Gr or compressing the underlying Ag/Re substrate, respectively. Different interface models and graphene-substrate distances were tested to determine the energetically most favourable placement of the carbon atoms relative to the substrate surface, yielding the top-fcc arrangement as the structure featuring the lowest energy. Due to interaction with the Ag/Re substrate, the electronic structure of graphene is modified, showing qualitative agreement with above mentioned ARPES experiments. We observe a downward shift of the Dirac point with respect to the Fermi energy as well as hybridization of the graphene π -band with the Ag d-bands. The strength of both phenomena depends on the graphene-substrate distance.

O 41.9 Wed 12:30 MA 041 Electronic spectrum and structure of an epitaxial graphene superlattice on SiC — •Konstantin Emtsev¹, Stiven Forti¹, CAMILLA COLETTI², and ULRICH STARKE¹ — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — $^2\mathrm{Center}$ for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy The electronic spectrum of graphene can be altered profoundly by the presence of an external potential that is periodic on an atomic scale [1]. Experimentally, such perturbations are sought after in graphene grown epitaxially on a crystalline substrate with commensurate or incommensurate lattice arrangements. In the present work we address the electronic and structural properties of such a graphene superlattice realized on a SiC substrate. We utilize the atomic intercalation phenomenon established earlier [2, 3] in order to create a new heterointerface graphene/copper/SiC. The samples were characterized by high resolution ARPES, XPS and LEED. As observed by LEED, the modified interface imposes a new long range reconstruction on graphene as opposed to as-grown epitaxial graphene on SiC. Changes in the electronic valence band spectrum of the graphene film detected by ARPES are related to a structural transformation of the graphene layer that we derive from XPS core level spectra. We compare our data to other epitaxial graphene systems and theoretical predictions.

[1] C.H. Park et al., Nat. Physics, 4, 213 (2008) [2] I. Gierz et al., Phys. Rev. B, 81, 235408 (2010) [3] K.Emtsev et al., Phys. Rev. B, 84, 125423 (2011)

O 41.10 Wed 12:45 MA 041 Interaction of hydrogen with graphene on Silicon carbide: un-DFT study of the electronic structure of graphene/Ag(111)/Re(0001) eling the interface structure – \bullet FRANCOIS C. BOCQUET^{1,2,4}, REGIS BISSON³, THIERRY ANGOT³, and JEAN-MARC THEMLIN^{1,2} -¹Aix-Marseille Université, IM2NP, France — ²CNRS, IM2NP (UMR 6242) F-13397 Marseille CEDEX 20, France — $^3\mathrm{PIIM},~\mathrm{UMR}$ 6633 CNRS-Université de Provence, F-13397 Marseille CEDEX 20, France ⁴Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA Fundamentals of Future Information Technology, 52425 Jülich, Germany

> Since the stability of a single graphene layer has been discovered, much effort was devoted to the thermal growth of graphene over SiC. Recently, the reversible adsorption of atomic hydrogen on graphene was shown to induce drastic changes in electronic properties between clean, low [1] and high coverages [2]. Also, at high temperature, hydrogen penetrate beneath the buffer layer resulting in free-standing graphene [3]. We studied the buffer layer forming prior to graphene growth on SiC(0001) as well as a single-layer of free standing graphene obtained by hydrogen intercalation. By a subtle tuning of graphene electronic properties with hydrogen adsorption, High Resolution Electron Energy Loss Spectroscopy (HREELS) is allowed to probe below the graphene sheet. This reveals unambiguously the nature of the covalent bond between SiC and the buffer layer.

> References [1] Bostwick, Phys. Rev. Lett., 103 (2009) 056404 [2] Elias, Science, 323 (2009) 610 [3] Riedl, Phys. Rev. Lett., 103 (2009) 246804