O 64: Poster: Graphene

Time: Wednesday 18:00–20:00 Location: P2/EG

O 64.1 Wed 18:00 P2/EG

An STM and XPS study of graphene on Rh (111) as a substrate for on-surface assembly of Pt-complexes — •Majid Shaker, Natalie J. Waleska, Simon Jaekel, Eva Marie Freiberger, Valentin Schwaab, Felix Hemauer, Rajan Adhikari, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, Erlangen 91058, Germany

Single platinum atoms have interesting properties and can play an important role in on-surface catalysis. One route to prepare small Pt nanoclusters or even single isolated Pt atoms is to deposit small amounts of Pt on the Moiré structure of 2D materials on lattice-mismatched transition metal surfaces. Such Moiré patterns e.g. of graphene can act as template for the formation of NCs with a narrow size distribution. In this study, a monolayer of graphene was successfully grown on the surface of a Rh(111) single crystal from ethylene (C2H4) as precursor under ultra-high vacuum (UHV). Very small Pt NCs (down to individual atoms) were formed in the valleys of graphene to further act as a transition metal center for the formation of metal complexes by providing appropriate ligands. Scanning tunneling microscopy and synchrotron radiation-based X-ray photoelectron spectroscopy were employed to evaluate the formed inorganic complexes.

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O 64.2 Wed 18:00 P2/EG

Graphene on Ru(0001): Layer-Specific and Moiré-Site- Dependent Phonon Excitations — Johannes Halle, Nicolas Néel, •Rebecca Cizek, and Jörg Kröger — Technische Universität Ilmenau

Graphene phonons are excited by the local injection of electrons and holes from the tip of a scanning tunneling microscope. Despite the strong graphene-Ru(0001) hybridization, monolayer graphene unexpectedly exhibits pronounced phonon signatures in inelastic electron tunneling spectroscopy. Spatially resolved spectroscopy reveals that the strength of the phonon signal depends on the site of the moiré lattice with a substantial red-shift of phonon energies compared to those of free graphene. Bilayer graphene gives rise to more pronounced spectral signatures of vibrational quanta with energies nearly matching the free graphene phonon energies. Spectroscopy data of bilayer graphene indicate moreover the presence of a Dirac cone plasmon excitation.

O 64.3 Wed 18:00 P2/EG

DFT study on the ORR mechanism on carbon nitride materials — •Jana Koenigsdorff, Changbin Im, Björn Kirchhoff, and Timo Jacob — Ulm University, Institute of Electrochemistry, D-89081 Ulm

Polymeric carbon nitrides (PCNs) have rapidly gained attention over the last years due to their promising physicochemical properties.[1] With their adjustable narrow bandgap and high visible light responsivity, PCNs are considered as promising potential photo-(electro)-catalysts for various industrial processes such as H_2O_2 formation or CO_2 reduction.[2][3] However, numerous structural and photophysical properties of this material class are not completely understood and hinder in-depth comprehension of the reaction pathways.[2] Most simulation studies that attempted to gain a deeper insight into the reaction mechanisms were based on simple, highly ordered PCN models.[1] However, PCNs obtained by thermal processes often exhibit inhomogeneity and a variety of micro-structural motifs.[2] In this study, we therefore perform DFT calculations to investigate the mechanism of H_2O_2 formation with various PCN models of different degrees of condensation and structural composition in order to screen a wide range of adsorption sites. We are convinced that with this approach, we can establish structure-reactivity relationships that can be used to derive understanding-driven material optimization strategies.

[1] Wei, Z. et. al., *Energy Environ. Sci.* **11** (2018) 2581 - 2589. [2] Lau, V. Lotsch, B., *Advanced Energy Materials* **12** (2022) 2101078. [3] Xia, Y. et. al., *ChemSusChem* **13** (2020) 1730 - 1734.

O 64.4 Wed 18:00 P2/EG

Electronic magneto-transport in epitaxial graphene covered with Bi(110) islands — •Sergii Sologub[1,2], Julian Koch[2], Chitran Ghosal[2], and Christoph Tegenkamp[2] — [1]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv — [2]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz

Magneto-conductance and Hall voltage of epitaxial graphene formed on SiC and covered with ultrathin Bi islands were measured within the range of ±4 T. The structure and morphology of Bi coverages of average thickness up to 4 bilayers, MBE-grown at RT as well as after-annealed, were determined by SPA-LEED and STM techniques. The coverage was found to consist of needle-like (110) islands with "magic" widths and thicknesses.

The analysis of the low-field part of the magneto-conductance reveals a transition from weak-localization (WL) to weak antilocalization (WAL) with increasing Bi coverage and allows to characterize the scattering of conduction electrons by determining electron scattering lengths, namely inelastic-dephasing, intervalley and intervalley symmetry breaking ones. The correlation of the average sizes of and distance between Bi(110) islands for different coverages with the characteristic lengths demonstrate the role of electron scattering on edges and within the islands in the WL-WAL transition. Calculated dependencies of Hall and magneto-resistance allow determining changes of the electron density induced by Bi adsorption and reveal the contribution of electron-electron interaction in electronic transport.

O 64.5 Wed 18:00 P2/EG

Organic Molecules on Graphene grown on a Pt(111) surface — •Shilpa Panchami Raj, Christophe Nacci, and Leonhard Grill — University of Graz

Graphene, a flat monolayer of carbon atoms with two-dimensional honeycomb lattice, exhibits unique properties. If grown on a Pt(111) surface, only weak interaction is found between the substrate and the graphene sheet. This renders it an interesting system to decouple organic molecules on the graphene layer from the metal underneath as they might preserve their electronic structure In this work, we present a scanning tunneling microscopy (STM) study under ultrahigh vacuum (UHV) with the deposition of different organic molecules on graphene that was epitaxially grown on a Pt(111) substrate. Experiments were done at cryogenic temperatures of 5 K, which allows to image single molecules in a stable fashion and also to manipulate them with the tip of the STM in a controlled way. Adsorption properties of the molecules are studied in view of the characteristic Moiré pattern of the graphene/Pt(111) system. Moreover, first attempts will be presented how chemical reactions can be induced on this system.

O 64.6 Wed 18:00 P2/EG

Electronic band structure of Pb intercalated graphene on SiC and the influence of electron doping — •Bharti Matta[1], Philipp Rosenzweig[1], Kathrin Küster[1], Craig Polley[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]MAX IV Laboratory, Lund University, Fotongatan 2, Lund 22484, Sweden

Intercalation is a powerful way of modifying the properties of epitaxial graphene and stabilizing two-dimensional (2D) intercalant layers at the graphene/SiC interface. In this work, we show that the charge neutrality of Pb intercalated quasi-freestanding monolayer graphene on SiC involves charge transfer from both the intercalant and the substrate. Synchrotron based angle resolved photoelectron spectroscopy measurements demonstrate the (1×1) order of the Pb layer with respect to SiC. The interlayer bands cross the Fermi level, confirming the metallic nature of intercalated Pb. Furthermore, constant initial state mapping shows no dispersion of the Pb bands with photon energy, proving the 2D nature of the intercalant layer. Polarization dependent measurements retrieve a mainly in-plane orbital character for the Pb band branches closer to the Fermi energy. Potassium deposition induces strong n-doping in the graphene layer ($E_D \approx 1.1$ eV). However, the Pb bands do not show any noticeable change, which suggests that the charge transfer from the potassium layer occurs predominantly into the graphene. Supported by DFG through FOR 5242.

O 64.7 Wed 18:00 P2/EG

Terahertz harmonic generation from graphite pencil drawings — •Atiqa Arshad, Segey Kovalev, and Jan Christoph —

Helmoltz Zentrum Dresden (HZDR)

Harmonic generation is a general characteristic of driven nonlinear systems. It can serve as an efficient tool for investigating the fundamental principles that govern the underlying ultrafast nonlinear dynamics. Here we report on terahertz third harmonic generation (THG) from graphite pencil drawings on paper. We demonstrate that the terahertz(THz)-THG efficiency at an excitation frequency of 0.5 THz in graphite is comparable to that of single-layer graphene pump field strengths on the order of 100 kV/cm-1. The THG efficiency in graphite exhibits a significantly less pronounced saturation behavior at high incident fields and thus may even surpass that of graphene at extreme pump field strengths. The less pronounced saturation can be attributed to more efficient heat dissipation in multilayer graphite flakes compared to single-layer graphene. The feasibility of using easy-to-produce graphite-based structures opens up new possibilities for highly accessible, modifiable, and nearly cost-free THz frequency multipliers. Besides the implementation of graphite-based THz frequency converters, the developed technique could be used for nonlinear THz imaging, offering the possibility to image graphite drawings covered by other materials.

O 64.8 Wed 18:00 P2/EG

In-situ monolayer graphene growth on Ru($10\bar{1}0$): an electron microscopy study — •Cathy Sulaiman, Lukas Schewe, Lars Buss, Moritz Ewert, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

During the last decade, the controlled growth of monolayer (MLG) and bilayer graphene has extensively been studied on the hexagonal Ru(0001) surface, which is a system that is known to form strong chemical bonds at the metal-graphene interface. Yet, little attention was paid to the influence of the substrate orientation that was demonstrated to have a significant impact for graphene growth on the Ir(001) and Ir(111) surfaces, the latter exhibiting a weak coupling between the graphene and the support. Therefore, in this study we have grown graphene on the rectangular Ru($10\bar{1}0$) surface by segregation and ethylene-supported chemical vapor deposition. A photoemission and low-energy electron microscope (PEEM & LEEM) has been utilized to directly characterize the MLG growth process with respect to variations in substrate temperature and step orientation. The expansion of the MLG islands is compared to the well-established carpet-growth mode on the Ru(0001) surface. These results have been complemented by probing of the occupied and unoccupied electronic structure of the islands using PEEM and intensity-voltage LEEM. Furthermore, the existence of two preferential surface reconstructions is identified via micro-illumination low-energy electron diffraction (LEED), whose spatial distribution is revealed by employing dark-field LEEM imaging.

O 64.9 Wed 18:00 P2/EG

Band structure and charge carrier dynamics of a Pb-intercalated graphene sheet on Ni(111) — •Eva Sophia Walther[1], Katharina Hilgert[1], Christina Schott[1], Sebastian Hedwig[1], Ka Man Yu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern, Germany — [2]Institute of Physics, Material Science in Mainz, JGU Mainz, Germany

The discovery of graphene acted as a starting point for the vast research field of 2D materials. However, on metal surfaces, most of the enthusiasm for exploring graphene's unique properties has been tempered by the strong interaction with its substrate, which results in severe changes in its electronic properties. One way to reduce the graphene-surface interactions is the intercalation of heavy metal atoms between the graphene and the underlying substrate. In our work, we use the highly reactive Ni(111) surface as a graphene substrate. On this surface, the linear dispersion of the Dirac cone is severely distorted and the K-point is located far below the Fermi energy. Here, we will show that Pb intercalation recovers the linear dispersion of the free-standing graphene. Using time- and momentum-resolved photoemission, we will further determine the influence of the Pb intercalation for the ultrafast charge carriers dynamics at the K-point of the Gr/Ni(111) interface.

O 64.10 Wed 18:00 P2/EG

Controlled fabrication of the graphene/Mn_5Ge_3 interface via Mn intercalation — •Vivien Enenkel[1], Yuriy Dedkov[2], Elena Voloshina[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, Universtätsstraße 10, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

Mn-based intermetallic compounds have recently been in focus of intensive research owing to their outstanding magnetic properties. In particular, epitaxial Mn_5Ge_3/Ge interfaces [1] are regarded to have the potential for the realization of efficient spin injection and manipulation in semiconductor structures compatible with the existing Si technology. Furthermore, for graphene on Mn_5Ge_3 an exchange splitting of the π states is predicted, with the two spin channels exhibiting a large difference in charge carrier mobility [2]. Here, we report on the fabrication of epitaxial graphene/Mn_5Ge_3 by Mn-intercalation at the graphene/Ge(110) interface, initially prepared by atomic carbon deposition on Ge(110) [3]. Depending on the sample temperature different phases can be generated, including Mn_5Ge_3, whose structure and electronic properties are studied by low-temperature scanning tunneling microscopy and spectroscopy.

[1] Y. Dedkov *et al.*, J. Appl. Phys. 105, 073909 (2009).
[2] E. Voloshina and Y. Dedkov, J. Phys. Chem. Lett. 10, 3212 (2019).
[3] J. Tesch *et al.*, Carbon 122, 428-433 (2017).

O 64.11 Wed 18:00 P2/EG

Force-Field Development for Graphene-Graphite Water Systems — •Otto Schullian and Roland Netz — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The wetting behavior of water on graphene/graphite surfaces is strongly dependent on the force fields chosen for the water-carbon interaction. Previously developed force fields were optimized to reproduce a specific contact angle for water on graphite (in the range of 85° to 95°). However, experiments show that the contact angle for water on graphite depends strongly on the preparation of the surface; they suggest that freshly exfoliated graphite has a surprisingly hydrophilic contact angle of 60°±13°, whereas old and potentially contaminated graphite surfaces are much more hydrophobic. For graphene the variance in contact angle is even more dramatic, ranging from 10° to 127°.

Here, we simulate contact angles for a range of water-carbon interaction strengths for one to five layers of graphene to provide the necessary parameters for a whole range of contact angles (30°-115°). In this way, one can tune the wetting behavior in simulation. From our results, we see that the graphene with no underlying support has a contact angle 2°-20° higher than the corresponding graphite system depending on the interaction strength. In addition, we investigate the frequency-dependent friction on flat graphene and graphite as a function of the interaction strength and the number of graphene layers via the Green-Kubo relation including a hydrodynamic correction.

O 64.12 Wed 18:00 P2/EG

Raman features of graphene and Weyl semimetals beyond the standard nonadiabatic theory — •Nina Girotto and Dino Novko — Institute of Physics, Zagreb, Croatia

Although graphene has already been thoroughly studied with Raman spectroscopy, there still exists a disagreement about the broadening mechanisms of the E2g mode and its actual temperature dependence [Nano Lett. 10, 466 (2010)]. Along with the importance of the nonadiabatic effects in graphene, higher order electron-phonon scattering processes also significantly impact the phonon spectrum. Specifically, the electron-phonon-induced lifetime and energy renormalization of the electron-hole pair excitations bring additional temperature dependence in the electron-coupled phonon modes and their corresponding linewidths. The nonadiabatic theory relying on first principles calculations, developed in [Phys. Rev. B 98, 041112(R) (2018)], is here successfully applied to graphene in various doping regimes and to Weyl semimetals, which contain a 3-dimensional analog of Dirac points in the electron band structure and are, therefore, excellent candidates for achieving a nonadiabatic regime.