O 6: Graphene: Electronic properties, structure and substrate interaction I (joint session O/TT)

Time: Monday 10:30–13:15 Location: MA 043

O 6.1 Mon 10:30 MA 043

A Molecular Model System for 5-7 Defects in Graphene — •Benedikt P. Klein[1], Markus Franke[2], Claudio K. Krug[1], Stefan R. Kachel[1], Phil Rosenow[1], Francois Posseik[2], Martin Schmid[1], Reinhard J. Maurer[3], Ralf Tonner[1], Christian Kumpf[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Department of Chemistry, University of Warwick, United Kingdom

The electronic and mechanical properties of graphene are strongly influenced by the presence of defects. One important type of defect is the 5-7 motif with a 5-membered ring adjacent to a 7-membered ring. Little is known about the interaction of 5-7 defects with an underlying substrate. In this study, we have obtained insight into this interaction by using molecular model systems. As a model for the 5-7 defects we use azulene, which is a bicyclic aromatic compound with a 5- and a 7-membered ring, while naphthalene is used as a model for the regular 6-6 motif. We investigated both molecules on Cu(111) and Ag(111) using PES, NEXAFS, TPD, scanning probe and NIXSW experiments. To deepen the understanding of the occurring interactions between molecule and surface, periodic DFT calculations were performed. The more localized frontier orbitals of azulene result in a much stronger and more localized interaction with the Cu(111) surface. This leads to interfacial charge transfer in the former LUMO and substantial in-plane and out-of-plane deformations, as well as a much smaller adsorption height.

O 6.2 Mon 10:45 MA 043

The Effect of Carbon 1s Core Hole on the Polarization Spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Our band structure calculations show a good agreement with experimental polarization spectra [1] across the carbon 1*s* edge of highly oriented pyrolytic graphite. The change of polarization characteristics upon reflection of linearly polarized synchrotron radiation as the huge rotation of polarization plane of up to 140° and the change to nearly fully circularly polarized light can be resembled good, showing best results for not full but partially core hole per excitation. The contributions from the *A* and *B* site of HOPG are discussed as well as the amount of electron removed from core state.

References: 1. C. Jansing et al, PRB **94**, 045422 (2016).

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O 6.3 Mon 11:00 MA 043

Giant magneto-photoelectric effect at a graphene edge — •Friedemann Queisser, Jens Sonntag, Annika Kurzmann, Martin Geller, Sascha Lang, Axel Lorke, and Ralf Schützhold — Fakultät für Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

Graphene is a promising material for optical or infrared absorption, as its pseudo-relativistic energy-momentum relation allows for a broad absorption bandwidth. In [1] we studied the charge separation at a graphene edge via a strong magnetic field. Motivated by the proposed mechanism, a surprisingly high magneto-photocurrent was measured in suspended graphene [2]. The observed photo-responsitivity (100 incident photons create up to 17 particle-hole pairs) strongly exceeds the predicted value. A possible mechanism to explain the large observed current is Auger-type scattering. The strong Coulomb interaction, $\alpha_{\text{graphene}} \gg \alpha_{\text{QED}}$, together with the enlarged phase space at the graphene edge lead to a large probability per unit time for the secondary particle-hole pair creation. We discuss various aspects of Auger-type scattering at the graphene edge.

References:

[1] F. Queisser and R. Schützhold *Phys. Rev. Lett.* **111**, 046601 (2013)

[2] J. Sonntag, A. Kurzmann, M. Geller, F. Queisser, A. Lorke, R. Schützhold, *New. J. Phys.* **19** 063028 (2017)

O 6.4 Mon 11:15 MA 043

Synthesis of two-dimensional materials using liquid metal catalysts: Instrument development for *in situ* studies — •Amirmehdi Saedi[1], Marc de Voogd[2], Arthur Sjardin[2], Gertjan van Baarle[2], and Irene Groot[1] — [1]Catalysis and Surface Chemistry, Leiden Institute of Chemistry, Leiden University, The Netherlands — [2]Leiden Probe Microscopy BV, Leiden, The Netherlands

Two-dimensional materials (2DMs), e.g. graphene, hold great promise for future applications in many technological areas. The current state-of-the-art synthesis method of these materials involves the dissociative adsorption of gas-phase precursors on a solid catalyst. This process is slow by nature, inefficient, and environmentally unfriendly. Using liquid metal catalysts (LMCats) instead of solid ones bears the prospect of a continuous production of 2DMs with unprecedented quality and production speed. The aims of this multinational collaborative project are to develop instrumentation capable of studying the ongoing chemical reactions on a LMCat, *in situ* investigations on its catalytic activity, and unraveling the growth mechanisms of 2DMs on surfaces of LMCats. Gaining this knowledge would be the key toward establishing the first efficient mass production method for 2DMs using this new technology. (Visit http://lmcat.eu/ for more info)

O 6.5 Mon 11:30 MA 043

Effects of bi-axial strain on heterostructure of hBN and graphene — •Francesco Delodovici[1], Silvana Botti[2], and Giovanni Onida[1] — [1]Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy — [2]Institute of Condensed Matter Theory and Optics Max-Wien-Platz 1 07743 Jena Germany

I will present a theoretical/computational study of the mechanical and electric properties of an heterostructure consisting of graphene superimposed to hexagonal boron nitride (hBN) when external biaxial strain is applied.

As a preliminary case, we consider a free-standing layer of hBN under uniform biaxial strain: we predict new thermodinamically stable configurations and analyze their mechanical properties, to understand whether they could be accessible experimentally. In addition, we characterize their electrical and optical properites, to detect the emergence of radical changes in hBN properties.

Further on, we turn our attention to the effects of equi-biaxial strain on the graphene-hBN heterostructure.

We use ab-initio crystal structure prediction, and more precisely the fixed-volume minima hopping method to sample the configuration space searching for new configurations. We use density functional tight binding methods to obtain energies and forces for structural prediction and DFT to characterize the electric properties of the new phases.

O 6.6 Mon 11:45 MA 043

Light-field-driven currents in graphene — •Christian Heide, Takuya Higuchi, Konrad Ullmann, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Strong-field physics centres on controlling the motion of electrons by virtue of an optical electric field with attosecond (10^{-18} s) precision. Graphene is an ideal playground for extending the scope of strong-field phenomena to a conductor because of its excellent carrier mobility, much weaker screening due to a low carrier concentration compared with conventional metals and its ultrafast and broadband optical response.

We will show that one can control the residual conducting current in epitaxially grown graphene by tailoring the electric-field waveform of few-cycle laser pulses, on attosecond timescales [1]. We interpret the waveform-dependent conducting current by considering graphene as a simple two-band system, interacting with an oscillating optical field of

an ultrashort laser pulse. We found a transition from the weak, perturbative nonlinear response (photon-driven) to optical-field-driven, nonperturbative electron dynamics, in which the influence of the intraband dynamics to the interband transition cannot be neglected. Inthis strong-field regime, electrons exhibit quantum-mechanical interference known as Landau-Zener-Stückelberg interference.

[1] T. Higuchi, C. Heide, K. Ullmann, H. B. Weber, and P. Hommelhoff, Light-field-driven currents in graphene, Nature 550, 224 (2017).

O 6.7 Mon 12:00 MA 043

Can the Coulomb interaction be added to the Dirac-Weyl equation of graphene? — •Fabian Rost and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen, Germany

On the basis of an exact operator equivalence between a lattice tight binding model and a continuum description $H(\mathbf{r},\mathbf{p})$ [1], we address the question of the required form the interaction potential $V_{eff}(\mathbf{r},\mathbf{r}')$ should take in the continuum description in order to maintain operator equivalence with the tight-binding Hamiltonian in the presence of an interaction potential $V(\mathbf{r},\mathbf{r}')$. To lowest order we find the natural answer: that $V_{eff}(\mathbf{r},\mathbf{r}') = \mathbf{V}(\mathbf{r},\mathbf{r}')$ but also that this is sufficient only in the case that $V(\mathbf{r},\mathbf{r}')$ does not change on the scale of the lattice constant. Taking the example of graphene we derive the corrections to the lowest order result for the case of the Coulomb interaction.

[1] N. Ray et al., arXiv preprint arXiv:1607.00920, 2016

O 6.8 Mon 12:15 MA 043

Optical deformations in graphene — •Reena Gupta and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Deformations in graphene slow on the scale of the lattice constant are, at lowest order, very well described by the addition of a pseudo-magnetic gauge field to the Dirac-Weyl equation [1]. Here we explore what happens when we consider slow deformations but of both possible modes that the two-atom unit cell allows, i.e., optical as well as acoustic modes. While the acoustic mode simply reproduces the well-known pseudo-magnetic gauge field, the optical mode generates both a chiral field as well as an imaginary magnetic gauge, with Hermiticity of the Hamiltonian maintained by a position dependent velocity correction. We comment on the relevance of these results to hybrid metal/graphene systems which feature strong deformation.

[1] B. Amorim et al., Physics Reports 617, 1 (2016).

O 6.9 Mon 12:30 MA 043

Moiré ordered current loops in the graphene twist bilayer — •Dominik Weckbecker and Sam Shallcross — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Moiré lattices in layered two dimensional materials possess, in the presence of a magnetic field of 1-5 Tesla, comparable structural and magnetic length scales and, as a consequence, exhibit remarkable magnetic field phenomena such as the recently observed Hofstadter butterfly [1,2].

In this contribution, we present the results of our simulations on twisted bilayer graphene nanoribbons, which were conducted using a semi-empirical tight-binding method [3].

We report novel phenomena arising from this interplay of length scales in the form of an ordered array of permanent current loops throughout a moiré generated by twisting graphene layers [3,4]. Strikingly, these current loops are found at significantly weaker fields than those required to observe the Hofstadter butterfly, and such current loops thus represent an additional low field imprint of the moiré lattice on Landau physics, and an unusual situation in which the field induced currents are found in the bulk of a material.

[1] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976)
[2] C. R. Dean et al. , Nature 497, 598-602 (2013)
[3] W. Landgraf et al., Phys. Rev. B. 87, 075433 (2013)
[4] manuscript in preparation

O 6.10 Mon 12:45 MA 043

A novel delocalized phase in the small angle graphene twist bilayer — •Maximilian Fleischmann, Reena Gupta, Dominik Weckbecker, and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

In this work we demonstrate that the small angle limit of the graphene twist bilayer contains, in addition to its well known localized phase [1], a novel delocalized phase accessible by applied interlayer bias. This phase differs profoundly from the large angle delocalized phase as, in contrast to the almost perfectly circular Fermi surface found at large angles, one finds almost perfectly linear Fermi lines. These may be translated into each other by a so-called nesting vector, the magnitude of which is controllable by the applied field. The finding of a phase in the twist bilayer consisting solely of one dimensional Fermi lines connected by field tunable nesting vectors, marks this system out as an unexpected playground for the study of nested Fermiology and electronic instabilities.

[1] D. Weckbecker et al., Phys. Rev. B **93**, 035452, 2016.

O 6.11 Mon 13:00 MA 043

Electronic and geometric structure of PTCDA films adsorbed on Graphene passivated Ni(111) — •Dominik Jungkenn[1], Johannes Seidel[1], Florian Haag[1,2], Leah L. Kelly[1], Mirko Cinchetti[3], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund

Organic molecules are highly intriguing materials for spintronics due to their wide range of functionalities. However, to take full advantage of these functionalities, ferromagnetic surfaces have to be passivated , either by an organic buffer layer or by an inert 2D material [1]. Along these lines, we have investigated the geometric and electronic structure as well as the hot electron dynamics of a PTCDA monolayer on a Graphene (Gr) passivated Ni(111) surface. We find the formation of long-range ordered PTCDA monolayer films on Gr/Ni(111) resembling the herringbone structure of PTCDA/Ag(111). The frontier molecular states reveal the orbital emission pattern of unperturbed PTCDA molecules suggesting, as expected, a weak coupling of the molecular layer to the Graphene sheet. [1] Cinchetti et al. Nat. Mater. 16, 507 (2017)