O 28: Moire and Graphene Stacking

Time: Tuesday 14:00–16:00 Location: MA 041

O 28.1 Tue 14:00 MA 041

Periodic Overlayers and Moiré Patterns: a unified theoretical treatment. — •Klaus Hermann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin (Germany)

Complex overlayer structures at single crystal surfaces have been observed where long-range order, expressed by additional approximate surface periodicity with very large unit cells, was found. Examples are Pb(111)-C_{60} near $(\sqrt{403}/7 \times \sqrt{403}/7)$R22.8° [1], Ag(111)-3S near $(\sqrt{7}\times\sqrt{7})$R19.1° [2], or graphene at different hexagonal metal surfaces, such as Ir(111) [3]. This phenomenon can be characterized by spatial interference resulting in 2-dimensionally periodic Moiré patterns. We have generalized a previously proposed mathematical formalism [4] of determining such Moiré patterns based on concepts of higher-order coincidence (HOC) lattices. The extended formalism provides simple mathematical relations allowing to compute 2-dimensional Moiré lattices of any order in their dependence on layer rotation and scaling with respect to a given HOC lattice structure. The formalism will be illustrated by example systems observed in experiment. [1] H.L. Li, K.J. Franke, J.I. Pascual, L.W. Bruch, R.D. Diehl, Phys. Rev. B **80** (2009) 085415. [2] M. Yu, D.P. Woodruff, C.J. Satterley, R.G. Joes, and V.R. Dhanak, J. Phys. Chem. **111** (2007) 3152. [3] E. Loginova, S. Nie, K. Thürmer, N.C. Bartelt, and K.F. McCarthy , Phys. Rev. B **80** (2009) 085430. [4] K. Hermann, J. Phys.: Condensed Matter 24 (2012) 314210.

O 28.2 Tue 14:15 MA 041

Semi-classical method for matrix valued Hamiltonians — •Michael Vogl, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik Staudtstr. 7-B2 91058 Erlangen

Semi-classical theories are interesting for their insight into the borderland phenomena embracing quantum and classical physics such as quantum chaos, as well as for providing a non-perturbative scheme for treating complex quantum problems. The plethora of complex graphene-based systems, such as the twist graphene bilayer consisting of two mutually rotated carbon layers, or the AB stacked bilayer with soliton faults (partial dislocations), are systems for which a semi-classical treatment should be very useful. However, the usual semi-classical schemes become prohibitively cumbersome for the matrix valued Hamiltonians inherent to the graphene-based systems. We provide a scheme that allows for a clear route to the semi-classical treatment of such systems, as well as a very efficient numerical scheme.[1] As an example of this procedure we consider the semi-classical treatment of a line partial dislocation in bilayer graphene.

[1] M. Vogl, Semi-classics for Matrix Hamiltonians, Master thesis, Erlangen, 2014.

O 28.3 Tue 14:30 MA 041

Scanning Probe Microscopy Study of Moiré Patterns on Rotated Graphene Layer on Highly Oriented Pyrolytic Graphite — •Dilek Yildiz[1,2], Şener Şen[3], Marcin Kisiel[1], Oğuz Gülseren[3], Ernst Meyer[1], and Oğuzhan Gürlü[2] — [1]University of Basel, Basel, Switzerland — [2]Istanbul Technical University, Istanbul, Turkey — [3]Bilkent University, Ankara, Turkey

Highly Oriented Pyrolytic Graphite (HOPG) has weak van der Waals interaction between its layers so they can be cleaved easily and fresh (0001) graphite surfaces can be obtained. As another result of this weak interaction, the topmost graphene layer can be rotated with respect to the rest of the crystal and super periodic structures called as moiré patterns are formed. Such moiré patterns were extensively studied by Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). In this study, we investigate the morphological and electronic properties of moiré patterns on HOPG by using STM and STS under ambient conditions. Apparent corrugation changes of different moiré patterns were studied as a function of the bias voltage. We studied the electronic properties of moiré patterns with respect to their periodicities. Van Hove singularities were observed on moiré patterns in STS data and their origin were clarified by means of ab initio calculations. Observation of moiré patterns by Atomic Force Microscopy (AFM) is yet to be reported on HOPG surfaces. In our recent studies we are interested in the frictional properties of varying moiré patterns on HOPG. Our particular interest is to observe the frictional response of the moiré patterns to the tip perturbation by use of pendulum geometry AFM.

O 28.4 Tue 14:45 MA 041

Low energy theory of the graphene twist bilayer — •Dominik Weckbecker, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik, Staudtstraße 7, D-91058 Erlangen, Germany

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle of the two layers. At large angles the layers essentially decouple while, in contrast, for small rotation angles strong coupling leads to a dramatically different electronic spectrum: one finds localization on the moire lattice and a significant reduction of the Fermi velocity near the Dirac point [1]. This richness of electronic structure has however proven difficult to capture within an unified low energy Dirac-Weyl picture; while theories exist for the large and small angle regimes there is at present no consistent theory valid at all twist angles [2,3]. We remedy this by deriving a low energy theory which is based on the observation of an emergent momentum coupling scale [1] valid at all angles, which we show to be in excellent agreement with numerical tight-binding calculations. We further explore the rich small angle limit finding a vanishing of the zero mode and a rich gallery of Fermi surfaces. At large angles the theory recovers the effective low energy Hamiltonians previously derived on symmetry grounds [3].

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013.
[2] R. Bistritzer et al., PNAS 108(30):12233-12237, 2011.
[3] E. J. Mele et al., J. Phys. D: Appl. Phys. 45 154004, 2012.

O 28.5 Tue 15:00 MA 041

What are the possible moiré patterns of graphene on hexagonally packed surfaces? - Universal solution for hexagonally packed coincidence lattices, derived by a geometric construction — •Patrick Zeller[1] and Sebastian Günther[2] — [1]Department Chemie, LMU, Butenandtstr. 5-13, D-81377 München — [2]Chemie Department, TUM, Lichtenbergstr. 4, D-85748 Garching

We performed a systematic investigation of two coinciding lattices and their spatial beating frequencies that lead to the formation of moiré patterns. A mathematical model was developed and applied for the case of a hexagonally arranged adsorbate layer on a hexagonal support lattice. In particular, it describes the moiré patterns observed for graphene (g) grown on hexagonally arranged transition metal surfaces, systems that serve as promising synthesis routes for the formation of this highly wanted material. We use a geometric construction that derives analytic expressions for first and higher order beating frequencies occurring for arbitrarily oriented g on an underlying substrate lattice. By solving the corresponding equations, we can predict the size and orientation of the resulting moiré patterns. Adding the constraints for commensurability delivers further solvable analytic equations that predict, whether or not first or higher order commensurable phases occur. We explicitly treat the case for first, second and third order commensurable phases. The universality of our approach is tested by comparing our data with moiré patterns that are experimentally observed for g-Ir(111) and g-Pt(111). The derived general properties of such patterns may be used to critically discuss reported moiré unit cells.

O 28.6 Tue 15:15 MA 041

Observation of Natural X-Ray Birefringence of Graphene — •Christine Jansing[1], Marc F. Tesch[1,2], Markus Gilbert[1], Andreas Gaupp[1], Hans-Christoph Mertins[1], Andrey Sokolov[2], Dong Hee Shin[3], Suk-Ho Choi[3], Heiko Timmers[4], Dominik Legut[5], and Peter M. Oppeneer[6] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]Research School of Physics and Engineering, Department of Electronic Materials Engineering, Australian National University, Canberra, ACT 0200, Australia — [4]School of Physical, Environmental and Mathematical Sciences, University of New South Wales Canberra, PO Box 7916, Canberra BC 2610, Australia — [5]Nanotechnology Centre, Ostrava, Czech Republic — [6]Depart. of Physics, Uppsala Uni., Box 530, S-751 21 Uppsala, Sweden

We present the first experimental results that demonstrate the x-

ray natural birefringence and the natural linear dichroism (XNLD) of graphene and compare these to our ab-initio calculations. The effects have been detected at the C 1s edge of a graphene monolayer on Cu using polarization spectroscopy in reflection with linearly polarized radiation at the UE56-2-PGM2 beamline at BESSY II. Upon reflection the polarization plane rotates showing an unusually large rotation value of 33° at the π*-states near 285 eV. Additionally the polarization of the light changes from linear to circular with a maximum value of Pcirc = 0.95. The new results for a monolayer graphene are compared with those obtained for highly-ordered pyrolitic graphite (HOPG).

O 28.7 Tue 15:30 MA 041

Reversible sublattice symmetry breaking in monolayer graphene nanomembranes using tip induced pseudomagnetic fields — •Alexander Georgi[1], Peter Nemes-Incze[1], Ramon Carillo-Bastos[2], Daiara Faria[2], Marco Pratzer[1], Ludger Wirtz[3], Nancy Sandler[2], and Markus Morgenstern[1] — [1]2.Physikalisches Institut B RWTH Aachen University — [2]Department of Physics and Astronomy, Nanoscale and Quantum Phenomena Institute, Ohio University — [3]Physics and Materials Science Research Unit, University of Luxembourg

Strain engineering in graphene might lead to a new generation of electromechanical devices, in particular due to its tunable pseudomagnetic field being a property of the unique sublattice degree of freedom within the honeycomb lattice. However, possibilities to tune the pseudomagnetic field on the nanoscale have not been realized so far. Here, we show that the forces of the tip of a scanning tunneling microscope can be used to switch local fields on and off, by applying strain, as visible by a relative change of the local density of states of the two sublattices up to 30 %. Comparison with tight binding simulations reveals that this contrast corresponds to a local pseudomagnetic field of up to 500 T.

We carefully rule out other possibilities for the apparent sublattice symmetry breaking such as buckling, a local Peierls transition, different lifting forces of the tip above different sublattices, or the correlation of electric and pseudomagnetic fields. Moreover, we show that model calculations of the van-der Waals forces between tip and graphene reproduce the observed effects quantitatively within 50 %.

O 28.8 Tue 15:45 MA 041

Electronic Conductivity of Twisted Bilayer Graphene — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

The electronic structure of a graphene twist bilayer in the small angle limit is characterized, for states near the Dirac point, by electron localization on the moire lattice and by a significant suppression of the band velocities [1]. This should lead to significant (and rotation angle dependent) changes of the bilayer conductivity. We explore this question within the low energy theory of the electron spectrum, and employing the linearized Boltzmann equation for the transport calculations [2]. We examine the scattering probabilities and the conductivity as functions of the twist angle, the doping level and the temperature. Our results show a dramatic decrease of the conductivity of a weakly doped bilayer with decreasing twist angle.

[1] S. Shallcross *et al.*, Phys. Rev. B **87**, 245403 (2013); [2] E. Mariani *et al.*, Phys. Rev. B **86**, 165448 (2012).