O 26: Transport: Graphene (TT jointly with O)

Time: Tuesday 9:30–13:15 Location: WIL C107

Topical Talk O 26.1 Tue 9:30 WIL C107

A First-Principles Perspective on Two-Dimensional Transition-Metal Dichalcogenides — •Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

Layered transition-metal dichalcogenides recently are attracting great attention, because of the possibility to achieve two-dimensional (2D) materials, similar to the exfoliation of graphene from graphite. Using first-principles calculations, we study prototypical monolayer MoS_2 to obtain insight into the influence of defects and substitutional doping, for a wide range of transition-metal dopants. We also address polar transition-metal dichalcogenide monolayers with respect to their structural stability and the effects of the spin-orbit coupling. Heterojunctions of MoS_2 with unsaturated and saturated MXenes are studied; such hyrid systems are interesting for application in all-2D devices.

[1] Phys. Rev. B 87, 100401(R) (2013)
[2] EPL 102, 57001 (2013)
[3] Phys. Rev. B 87, 245307 (2013)

O 26.2 Tue 10:00 WIL C107

Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institute of Nanotechnology (INT) and Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe Institut of Technologie (KIT), D-76131 Karlsruhe, Germany

Using our DFT-based transport framework AITRANSS [1,2], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen.

We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

As one expects, very wide ribbons (flakes, $W \gg L$) exhibit the bulk conductance $G = \frac{2e^2}{h}\frac{W}{\pi L}$ in the absence of adsorbants. With 20% hydrogen absorbants, we observe very complicated patterns of streamlines with many eddies and a broad distribution of local magnetic fields, $\mathbf{B}(\mathbf{r})$, that are induced by the dc-current flow. We plan to study the statistics of the conductance and $\mathbf{B}(\mathbf{r})$ of such large flakes and its dependency on the impurity concentration. Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we parallelized our transport module AITRANSS using standard MPI and OpenMP techniques, also including Scalapack to treat systems up to 10.000 carbon atoms.

[1] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).
[2] J. Wilhelm, MW, *et al.*, Phys. Chem. Chem. Phys. **15**, 6684 (2013).

O 26.3 Tue 10:15 WIL C107

Quantum transport simulations and Fabry-Perot interference patterns in multiple pn-junctions on graphene — •Fedor Tkatschenko[1], Ming-Hao Liu[1], Klaus Richter[1], Martin Drienovsky[2], Jonathan Eroms[2], and Dieter Weiss[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Advancements in experimental techniques have led to an amazing progress towards excellent graphene samples and to graphene devices with fascinating properties, ranging from narrow pnp junctions below 100 nm to large mean free paths up to micron scales. In such devices the charge carriers undergo multiple reflections at pn or np interface leading to interesting Fabry-Perot-type interference patterns in the conductance map[1,2]. We address the peculiar features of Fabry-Perot resonances in graphene. To this end we calculate the potential profiles for typical experimental setups[3] with the quantum capacitance model and perform transport calculations using the recursive Green's function technique. The numerical results are in good agreement with the experimental data. We further show that the leading contribution to the Fabry-Perot resonances in the conductance map originates from the first two pn junctions.

[1] A.F. Young and Ph. Kim, Nat. Phys. **5** (2009)
[2] P. Rickhaus, R. Maurand, M. H. Liu, M. Weiss, K. Richter and C. Schönenberger, Nat. Comm. **4** 2342 (2013)
[3] M. Drienovsky, F.-X. Schrettenbrunner, M. H. Liu, F. Tkatschenko, K.Richter, D. Weiss and J. Eroms, in preparation

O 26.4 Tue 10:30 WIL C107

Ballistic interferences in suspended graphene — •Ming-Hao Liu[1], Peter Rickhaus[2], Romain Maurand[2], Markus Weiss[2], Klaus Richter[1], and Christian Schönenberger[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Complex Fabry-Pérot interferences in ultraclean suspended graphene have been recently observed, with the ballistic origin confirmed by transport calculations well agreeing with experiment [1]. The observed conductance oscillations account for quantum interference of electron waves propagating ballistically over distances exceeding 1 μm. The complex interference patterns stem from Fabry-Pérot resonances within different cavities defined by electrically controlled pn junctions and the graphene-contact interfaces. In this talk, the theoretical part of this work [1], namely, the full modeling of the ballistic transport from contact to contact through the suspended graphene, will be illustrated at an appropriate depth.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nat. Commun. **4**, 2342 (2013)

O 26.5 Tue 10:45 WIL C107

Ballistic transport in graphene nanoconstrictions — •Danny J. M. Jörger[1,2], Bernat Terrés[1,2], Stephan Engels[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Slava V. Rotkin[1,4], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [4]Physics Department, Lehigh University, Bethlehem, Pennsylvania 18015, USA

Graphene nanodevices, such as for example nanoconstrictions are interesting systems for studying mesoscopic phenomena. Recent developments in the fabrication of graphene devices have revealed a significant increase in carrier mobility (e.g. 200.000 cm^2/Vs in bulk samples), making mean free path in the order of device dimensions accesible. This allows to investigate quantum interference effects and ballistic transport in nanostructured graphene. We discuss the differences in electrostatic coupling ($\alpha \approx 9.4 \times 10^{10}$ $cm^{-2}V^{-1}$) at high and low magnetic fields and the width-dependency of the overall conductance level at zero magentic field. Results confirm the Dirac fermion nature of confined charge carriers in graphene. We report on the observation of quasi one-dimensional subband transport characteristics in graphene nanoconstrictions encapsulated in hexagonal boron nitride. The ballistic nature of the transport in our devices ($l_m \geq 500$ nm) allows to study the interplay between confinement and Landau quantization and its crossover.

15 min. break.

O 26.6 Tue 11:15 WIL C107

Optical conductivity of graphene — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Graphene is a two-dimensional crystal of carbon atoms with a honeycomb structure, which has many fascinating optical and electronical properties. It has a high mobility of electrons at room temperature and a high transparency of light with 97.7%. In the optical domain, the value of the transparency does not depend on the frequency of white light being transmitted and is thus universal. This universality is linked to the fine structure constant $\alpha = 1/137$ and can be derived using non-interacting Dirac fermions.

We aim to understand the correction of the optical transparency due to Coulomb interaction. Since there is a long dispute about this correction in the literature [1-6], we try to resolve this controversy. Therefore we combine two different regularization schemes: dimensional regularization and a deformation of the Coulomb potential. We discuss the physical implication of the choice of the regularization.

[1] Herbut, Juricic, Vafek, Phys. Rev. Lett. **100**,046403 (2008)

[2] Mishchenko, Europhys. Lett. **83**, 17005 (2008)
[3] Sheey, Schmalian, Phys. Rev. B **80**, 193411 (2009)
[4] Juricic, Vafek, Herbut, Phys. Rev. B **82**, 235402 (2010)
[5] Rosenstein et al., Phys. Rev. Lett. **110**, 066602 (2013)
[6] Gazzola, Cherchiglia, Cabral, Nemes, Sampaio, Europhys. Lett. **104**, 27002 (2013)

O 26.7 Tue 11:30 WIL C107

Polycrystalline graphene: mechanical, electrical and thermal properties — •Thomas Lehmann[1,2], Arezoo Dianat[1,2], Frank Ortmann[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany

Large-area samples of graphene tend to be polycrystalline (PC) on some substrates. Grain boundaries with structural defects are expected to alter the structural and electronical properties of graphene. In this work, the mechanical properties of PC graphene are studied by means of density-functional theory and furthermore the electrical and thermal transport properties are addressed. To construct grain boundaries of zigzag and rotated armchair graphene sheets, molecular dynamics simulations are performed. The critical strain leading to structural failure of PC graphene nanoribbons is only half the value of pristine armchair nanoribbons. However we show that it can be significantly enhanced by the reaction of the chemically active grain boundaries with atmospheric gases. The transport properties of those systems are investigated, both parallel and perpendicular to the grain boundary, using an ab initio based atomistic model combined with Landauer transport theory and recursive Green function method. The electronic part is calculated within a tight-binding model and a force-constant approach has been applied for phonon transport.

O 26.8 Tue 11:45 WIL C107

Electric field control of spin-polarized electron transport through zigzag graphene nanosheets — •Dirk Wiedmann[1], Marius Bürkle[2], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the spin-polarized transport through a finite zigzag graphene nanoribbon, contacted by carbon-nanotube electrodes [1]. The electronic structure is determined from density functional theory, and Green's functions are used to compute the phase-coherent electric current within the Landauer scattering theory. We observe antiferromagnetically coupled edge states in the graphene nanosheet, which may lead to spin-polarized currents. We analyze how they depend on the position of the electrodes and on applied transverse electric fields. Our ab-initio results are rationalized with the help of a Hubbard model.
[1] D. Wiedmann, M. Bürkle, and F. Pauly, in preparation.

O 26.9 Tue 12:00 WIL C107

Radiative damping and synchronization in a graphene-based terahertz emitter — •Andrey Moskalenko and Sergey Mikhailov — Institute of Physics, University of Augsburg, Germany

We investigate the collective electron dynamics in a recently proposed graphene-based terahertz emitter [1] under the influence of the radiative damping effect, which is included self-consistently in a molecular dynamics approach. We show that under appropriate conditions synchronization of the dynamics of single electrons takes place, leading to a rise of the oscillating component of the charge current. The synchronization time depends dramatically on the applied dc electric field and electron scattering rate, and is roughly inversely proportional to the radiative damping rate that is determined by the carrier concentration and the geometrical parameters of the device. The emission spectra in the synchronized state, determined by the oscillating current component, are analyzed. The effective generation of higher harmonics for large values of the radiative damping strength is demonstrated.
[1] S. A. Mikhailov, Phys. Rev. B 87, 115405 (2013)

O 26.10 Tue 12:15 WIL C107

Non-vanishing Coulomb drag in clean double-layer graphene at the Dirac point — •Sven Aeschlimann[1], Michael Schütt[2], Igor Gornyi[1,2,3], Boris Narozhny[1], and Alexander Mirlin[1,2,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A. F. Ioffe Physica-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

Coulomb drag is the frictional effect of simple Coulomb interaction onto two currents driven through two spatially separated conducting layers. Initiating a current through one layer, causes a current or a voltage drop in the other.

Recent experiments revealed a suprising nonvanishing resistance at the Dirac point that was expected to be zero for symmetry considerations. We focus on the possibility of a non-vanishing resistance in clean samples due to third order interaction contributions to drag.

O 26.11 Tue 12:30 WIL C107

Linear Magnetoresistance in bilayer graphene — •Ferdinand Kisslinger, Christian Heide, Christian Ott, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, ferdinand.kisslinger@physik.uni-erlangen.de

We investigate the magnetoresistance in bilayer graphene obtained by hydrogen intercalation of monolayer graphene grown on the SiC(0001) surface. Whereas in monolayer graphene electron-electron-interaction and weak localization can be observed at low temperatures, a strong linear contribution dominates the magnetoresistance for bilayer graphene. It is found to be nearly temperature independent.

A variation of charge carrier density using a bottom gate and the comparison of different samples is carried out. The entity of data agrees well with a theoretical model [1] that describes a resistance network of Van-der-Pauw resistors. Consistency with the experiment is achieved when a network of resistors with different resistances is assumed. There are several possibilities where such inhomogeneities may originate from. We can exclude some of them and propose dislocations recently found in bilayer graphene [2] as a good candidate causing this effect.
[1] M.M. Parish and P.B. Littlewood , Nature 426 (2003) 162
[2] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer and E. Spiecker, Nature (2013), accepted, DOI: 10.1038/nature12780

O 26.12 Tue 12:45 WIL C107

Wigner Crystal phases in bilayer graphene — •Peter Silvestrov and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig, Germany

It is generally believed that Wigner Crystal in single layer graphene can not exist because the magnitudes of the electron interaction and the kinetic energy scale similarly with the decreasing electron density. This scaling argument however does not work for the low energy states in bilayer graphene. We consider the Wigner Crystal in slightly doped bilayer graphene with a gap in spectrum opened by applying a perpendicular electric field. We argue that in this system the formation of the Wigner Crystal is not only possible, but a different phases of the crystal with very peculiar properties may exist here depending on the parameters.

O 26.13 Tue 13:00 WIL C107

Half-metallic bilayer graphene — •Jie Yuan — Raum 26 A 407 RWTH Aachen Sommerfeldstrasse 26, D-52056, Aachen

Charge neutral bilayer graphene has very likely a gapped ground state, as transport experiments have demonstrated. The nature of the ground state is undertermined yet. One plausible ground state is the layered antiferromagnetic spin density wave (LAF) state, where the spins in the top and bottom layers have the same magnitude with opposite directions. We propose that lightly doped bilayer graphene in an electric field perpendicular to the graphene plane may be a half-metal where only one spin direction lis conducting. By the special properties of the half-metal deriving from the LAF state, the primary source of the gap at charge neutrality may be distinguished from other competing ground states like the quantum spin-Hall state. We study this explicitly by using a mean-field theory on a two-layer Hubbard model.