

O 42: Graphene II

Time: Wednesday 11:15–12:45

Location: WIL B321

O 42.1 Wed 11:15 WIL B321

Graphene edge magnetism for spintronics applications: Dream or Reality? — ●JENS KUNSTMANN¹, CEM ÖZDOĞAN², ALEXANDER QUANDT^{3,4}, and HOLGER FEHSKE³ — ¹Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — ²Department of Computer Engineering, Cankaya University, Ankara, Turkey — ³Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Germany — ⁴School of Physics, University of the Witwatersrand, South Africa

We critically discuss the stability of edge states and edge magnetism in zigzag edge graphene nanoribbons (ZGNRs). We point out that magnetic edge states might not exist in real systems, and show that there are at least three very natural mechanisms – edge reconstruction, edge passivation, and edge closure – which dramatically reduce the effect of edge states in ZGNRs or even totally eliminate them. Even if systems with magnetic edge states could be made, the intrinsic magnetism would not be stable at room temperature. Charge doping and the presence of edge defects further destabilize the intrinsic magnetism of such systems. We conclude that edge magnetism within graphenes ZGNRs is much too weak to be of practical significance, in particular for spintronics applications. [1] J. Kunstmann, C. Özdoğan, A. Quandt, H. Fehske, arXiv:1007.2602 (2010).

O 42.2 Wed 11:30 WIL B321

Electronic properties of graphene superlattices in a strong magnetic field — ●GEORGE PAL, WALTER APEL, and LUDWIG SCHWEITZER — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

The application of 1-dimensional periodic potentials to graphene leads to new and unexpected phenomena. For example, new Dirac points are induced in the band structure whose positions are controlled by the ratio between the strength and the period of the superlattice potential. Also, the conductivity shows strong resonances when new zero energy states appear.

When graphene superlattices are placed in a magnetic field, the system is described by three length scales: the lattice constant, the period of the superlattice, and the magnetic length. When the parameters of the system are tuned such that these three characteristic lengths are commensurable, then the band structure is modulated in an unique way which has important consequences for the electronic and transport properties.

We study theoretically the electron properties of graphene superlattices in a perpendicular magnetic field within the lattice model. We show that the band structure changes dramatically depending on the ratio between the magnetic length and the superlattice period. Moreover, for certain strengths of the superlattice potential, additional energy gaps open in the Landau bands, which may lead to unusual plateau sequence in the Hall conductivity.

O 42.3 Wed 11:45 WIL B321

Mechanically-induced transport switching effect in graphene-based nanojunctions — TAKAZUMI KAWAI¹, MARKUS POETSCHKE², ●CLAUDIA GOMES DA ROCHA², YOSHIYUKI MIYAMOTO¹, STEPHAN ROCHE³, and GIANAURELIO CUNIBERTI² — ¹Green Innovation Research. Laboratoriess, NEC Corp., 34 Miyukigaoka, Tsukuba, Ibaraki, Japan — ²Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — ³Centre d' Investigació en Nanociència i Nanotecnologia (ICN-CSIC), UAB Campus, E-08193 Bellaterra, Spain

We present a theoretical study suggesting a novel type of electronic switching effect, driven by the geometrical reconstruction of nanoscale graphene-based junctions. We considered junction structures which have alternative metastable configurations transformed by rotations of local carbon dimers. The use of external mechanical strain allows a control of the energy barrier heights of the potential profiles and also changes the reaction character from endothermic to exothermic or vice-versa. The reshaping of the atomic details of the junction encode binary electronic ON or OFF states, with ON/OFF transmission ratio that can reach up to 100000. Our results suggest the possibility to design modern logical switching devices or mechanophore sensors, monitored by mechanical strain and structural rearrangements.

O 42.4 Wed 12:00 WIL B321

Charged collective excitations and SU(4) symmetry in graphene — ●ANDREA FISCHER¹, RUDOLF RÖMER¹, and ALEXANDER DZYUBENKO^{2,3} — ¹University of Warwick, Coventry, UK — ²California State University Bakersfield, California, US — ³General Physics Institute, Russian Academy of Sciences, Moscow, Russia

We show that graphene in a strong magnetic field with partially filled Landau levels sustains charged collective excitations, which are bound states of three-particle complexes [1]. Some of these states are optically bright and may be detected in spectroscopy experiments, enhancing the current understanding of electron-electron interactions in graphene. Indeed, such states have recently been seen at zero magnetic field in an ARPES study [2]. The states can be classified using the geometrical symmetries - non-commutative magnetic translations and generalized rotations - in addition to the dynamical SU(4) symmetry in graphene. From the SU(4) symmetry point of view, such excitations are analogous to bound states of two quarks and one antiquark with four flavours. Using Young diagram techniques, we determine the multiplet structure and establish a flavour optical selection rule to identify the bright states for experimental studies.

[1] A.M. Fischer, R.A. Römer and A.B. Dzyubenko, arXiv:1005.3277

[2] A. Bostwick *et al.*, Science **328**, 999 (2010)

O 42.5 Wed 12:15 WIL B321

Electronic structure of graphene twist stacks — ●SAM SHALLCROSS¹, SANGEETA SHARMA², and OLEG PANKRATOV¹ — ¹Lehrstuhl für Theoretische Festkörperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany. — ²Max-Planck Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany.

We present a study of graphene stacks consisting of an ordered sequence of pairs of twisted layers - the graphene twist stack; extending previous work on the graphene twist bilayer [1,2]. We find that this remarkable system entails a fundamental mixing of dimensionalities: while the twist stack spectrum is generated by an ensemble of *independent effective twist bilayer* Hamiltonians, the wavefunctions are products of *bilayer* wavefunctions and standing electron waves in the stacking direction, and thus extend over many layers of the stack. These have the property that of the ensemble of Dirac cones that constitute the twist stack band structure, it is those topologically closest to single layer graphene that dominate the surface region. We further examine the impact of stacking disorder, finding that these results are robust for moderate stacking fault density. With these results we are able to explain some of the striking differences between the physics of graphene grown on the C-face of SiC, and the by now well studied model of this system, the graphene twist bilayer.

[1] S. Shallcross, S. Sharma, E. Kandelaki, and O. A. Pankratov, Phys. Rev. B, 81:165105, 2010.

[2] S. Shallcross, S. Sharma, and O. A. Pankratov, Phys. Rev. Lett., 101:056803, 2008.

O 42.6 Wed 12:30 WIL B321

Selective chemisorption of graphene-like molecules on the Si(111) 7×7 surface: A theoretical study — ●JANOS KISS, THOMAS GRUHN, and CLAUDIA FELSER — Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

Graphene and porous graphene are very promising materials, which have been widely studied for electronic applications. Because of their improved properties, in the future it is expected, that graphene, porous graphene and graphene-like molecules will replace silicon. Despite its superior material properties, however, the field-effect transistors based on graphene or graphene nanoribbons build so far via top-down approaches have low on/off ratios. On the other hand, molecular nanotransistors build with precisely know atomic structures resembling graphene were synthesized only very recently. In order to pave the way towards the industrial fabrication of molecular nanotransistors, we have investigated the chemisorption of graphene-like molecules on the 7×7 reconstructed Si(111) surface via density functional theory (DFT) calculations. We found, that Si(111) is a very promising candidate to serve as substrate for the large-scale fabrication of coronene-based molecular transistors. Moreover, our calculations show, that various

adsorbate molecules prefer specific binding sites on the Si(111) surface. By following the template of the Si(111) substrate, the molecules se-

lectively adsorb and form a well defined two-dimensional grid with a 1×1 surface pattern.