# HL 22: Graphene: Structure and Theory II

Time: Monday 17:15–19:00 Location: EW 201

HL 22.1 Mon 17:15 EW 201

**DFT+CI calculations of quantum dots in graphene nanoribbons** — •Tobias Burnus[1], Gustav Bihlmayer[1], Daniel Wortmann[1], Ersoy Sasioglu[1], Stefan Blügel[1], and Klaus Michael Indlekofer[2] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Hochschule RheinMain, Unter den Eichen 5, 65195 Wiesbaden, Germany

Graphene nanoribbons (GNR) hold great future promise for field-effect transistors and quantum-dot devices. With gate electrodes an in-plane electric field can be generated, which localizes quantum-dot states in the bandgap of armchair GNR. Density-functional theory (DFT) calculations have been used to calculate GNR under an in-plane gate electric field, taking correctly the edge termination of the ribbon into account. The results obtained via DFT have been combined with the screened Coulomb interaction calculated within the random-phase approximation to setup a configuration interaction (CI) calculation for the quantum dot, which properly describes the multiplet states of the few electrons in the quantum dot. The results of this DFT+CI calculation can be used for a description of the time-dependent spin decoherence.

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HL 22.2 Mon 17:30 EW 201

**Universal infrared absorbance of 2D honeycomb crystals** — •Lars Matthes[1,2], Friedhelm Bechstedt[1], Olivia Pulci[2], and Paola Gori[3] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Dipartimento di Fisica, Università di Roma "Tor Vergata", via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]CNR-ISM, Via Fosso del Cavaliere 100, 00133 Rome, Italy

Recently it has been demonstrated experimentally that the optical transparency of graphene is only determined by the Sommerfeld finestructure constant $\alpha$. [1,2] This result is in agreement with the theory of non-interacting isotropic Dirac fermions with pseudospin and using the vector-potential gauge for the electromagnetic field. [1,3]

Using the complex dielectric function for optical interband transitions, we show the universal result that the low-frequency absorbance obtained for graphene also holds for the 2D group IV crystals silicene and germene, although they are not atomically flat. The result is derived by means of ab-initio electronic-structure calculations for two-dimensional crystals with honeycomb geometry without assuming chiral massless Dirac fermions. It does not depend on the group-IV atom, the sheet buckling, the orbital hybridization, and the gauge used to calculate the optical oscillator strength.

[1] R. R. Nair et al., Science 320, 1308 (2008)
[2] F. Maket al., Phys. Rev. Lett. 101, 196405 (2008)
[3] L. Yang et al., Phys. Rev. Lett. 103, 186802 (2009)

HL 22.3 Mon 17:45 EW 201

**Electronic Structure of Graphene Twist Flakes** — •Karla Türschmann, Wolfgang Landgraf, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen, Staudtstr. 7B2, 91058 Erlangen

The chemical exfoliation of graphene, that is the reduction of a highly ordered graphite crystal to single and multilayer graphene flakes via a wet chemical route, represents one of the most promising techniques for the mass production of high quality graphene. The bilayer flakes most probably consist of mutually rotated graphene layers, and in this work we describe the electronic properties of such systems. We use the tight-binding method in conjunction with Lanczos diagonalisation allowing us to access the required very large system sizes. For large twist angles we find an electronic decoupling of the flake layers, whereas for small angles we find a localisation of low energy quantum states associated with the moire pattern of AA and AB stacked regions of the twist flake.

HL 22.4 Mon 18:00 EW 201

**The Self-similar Limit of the Graphene Twist Bilayer: Zero Mode and Wavefunction Localization** — •Sam Shallcross and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen, Staudtstr. 7B2, 91058 Erlangen

The graphene bilayer consisting of mutually rotated layers shows a rich physics, including both a large angle electronic decoupling of the constituent layers, and a small angle regime characterised by an emergent length scale, the moiré length, and dramatic changes in the density of states near the Dirac point [1]. In this work we present tight-binding results for a complete range of twist angles ($\theta$), demonstrating the existance of a small angle limit in which the system becomes *self-similar* with $\theta$, i.e., reduction of $\theta$ leads to no changes in electronic properties when scaled by system size $N$. This regime is characterised by a zero mode consisting of states strongly localised on the AA patches of the lattice. In addition we present a low energy gauge theory of this self-similar regime, and demonstrate that it yields good agreement with the tight-binding results.

[1] S. Shallcross *et al.* Phys. Rev. B **81**, 165105 (2010)

HL 22.5 Mon 18:15 EW 201

**Electron Scattering by Buffer Layer Acoustic Phonons in Graphene on SiC Si-face** — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen, Staudtstr. 7B2, 91058 Erlangen

Graphene grown epitaxially on SiC presents one of the most promising routes towards the technological implementation of graphene, as well as being an interesting physical system in its own right. Key features of this system are a doping which places the Fermi level $\approx 450$ meV above the Dirac point, and a much reduced electron mobility ($\approx 3000$ cm$^2$/V.s at room temperature). In this work we describe a mechanism in which accoustic surface phonons modify the graphene-substrate separation resulting in a deformation potential and hence electron scattering. With this model we then calculate transport properties within the Boltzmann formalism, finding agreement with recent experimental work [1] demonstrating a remarkable *decrease* in the resistivity ($\rho$) near the Dirac with increasing temperature ($T$), a linear increase of $\rho$ with $T$ away from the Dirac point, and a good description of the graphene electron mobility.

[1] S. Tanabe *et al.* Phys. Rev. B **84**, 115458 (2011)

HL 22.6 Mon 18:30 EW 201

**Density Oscillations in a Graphene Bilayer** — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen, Staudtstr. 7B2, 91058 Erlangen

Density oscillations due to an impurity in graphene (Friedel oscillations) show a remarkable $1/r$ decay due to intervalley interference ($1/r^2$ is the expected envelope form for a two dimensional $e$-gas) [1]. In this work we describe Friedel oscillations in Bernal, AA, and twist graphene bilayers. We consider an ideal $\delta$-function impurity in conjunction with a low energy Green's function of the bilayer system, and solve the Dyson equation exactly. We find that in addition to the Friedel oscilations in the local density of states, there is an additional long period modulation resulting from the interlayer coupling. Furthermore, we find the magnitude of such density oscillations are substantially increased near the Dirac point in Bernal stacked graphene as compared to single layer graphene.

[1] C. Bena, Phys. Rev. Lett., 100, 076601 (2008)

HL 22.7 Mon 18:45 EW 201

**Graphene on Different SiC Polytypes** — Oleg Pankratov, •Stephan Hensel, and Paul Götzfried — Theoretische Festkörperphysik, Universität Erlangen, Staudtstr. 7B2, 91058 Erlangen

Epitaxial graphene grows on different SiC polytypes, yet the influence of the substrate polytype on graphene Dirac spectrum has not been systematically studied. We address this question with ab initio calculations, comparing the electronic structure of a graphene epilayer on polytypes with different hexagonality, various terminations and buffer/epilayer stackings within the $(\sqrt{3}\times\sqrt{3})$R30 interface model. We find the Dirac point alignment relative to the valence band substantially varies depending on polytype, but the Fermi level pinning and hence the doping of the epilayer stay the same. For the most relevant case of a buffer/epilayer Bernal stacking (Si-face) the Dirac cone splits by $\varepsilon_g < 40$ meV, whereas it remains intact for the AA-stack. This can be understood within the analytical symmetry-based model, which allows to establish a direct connection between $\varepsilon_g$ and the buffer/epilayer interaction potential.