O 16: Graphene: Theory (HL with O/TT)

Time: Monday 15:00–17:15 Location: ER 164

O 16.1 Mon 15:00 ER 164

The decoupling of epitaxial graphene on SiC by hydrogen intercalation: an *ab initio* study — •Lydia Nemec[1], Patrick Rinke[1,2], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Aalto University, Helsinki, Fi — [3]Duke University, Durham, NC, USA

Large-scale ordered epitaxial graphene can be grown on various substrates, out of which silicon carbide (SiC) is one of the most promising. The exact material properties of graphene depend on the growth conditions and its interaction with the substrate. By hydrogen intercalation of epitaxial graphene on the Si-face of SiC the graphene layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [1].

We performed an density functional theory study of QFMLG on the polar 6H-SiC(0001) surface based on a van der Waals corrected semi-local exchange-correlation functional using the all-electron numeric atom-centered basis function code FHI-aims. We find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene.

Using the insight gleaned on the Si-face, we present the structure of a hypothetical QFMLG phase on the C-face of SiC. We find that hydrogen intercalation is a promising option to control the SiC-graphene interface.

[1] C. Riedl, *et. al*, PRL 103, 246804 (2009).

O 16.2 Mon 15:15 ER 164

Two-dimensional analysis of the double-resonant 2D Raman mode in bilayer graphene — •Felix Herziger[1], Matteo Calandra[2], Paola Gava[2], Patrick May[1], Michele Lazzeri[2], Francesco Mauri[2], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]IMPMC, Université Pierre et Marie Curie, CNRS, 75252 Paris, France

The double-resonant 2D-mode Raman process in bilayer graphene has been discussed controversially in recent years. In this context, different models were proposed to explain the complex lineshape observed in experiments.

Using a two-dimensional first-principles calculation, we investigate the dominant contributions to the double-resonant Raman scattering cross-section of the 2D mode in bilayer graphene [1]. In contrast to previous works, we demonstrate that so-called 'inner' processes are, by far, the most dominant processes, as in single-layer graphene. Moreover, we show that the splitting between the two TO-derived phonon branches in bilayer graphene cannot be neglected for a consistent understanding of the 2D-mode lineshape. Additionally, we investigate the contributions from both TO branches to the symmetric and antisymmetric scattering processes. Our results answer the long-standing question regarding the different contributions to the 2D-mode lineshape in bilayer graphene.

[1] F. Herziger, M. Calandra, P. Gava, P. May, M. Lazzeri, F. Mauri, and J. Maultzsch, Phys. Rev. Lett. 113, 187401 (2014)

O 16.3 Mon 15:30 ER 164

Edge effects in the Raman spectra of atomically precise graphene nanoribbons: an ab-initio study — Marzio De Corato[1,2], •Deborah Prezzi[2], Alice Ruini[1,2], and Elisa Molinari[1,2] — [1]Department of Physics, Mathematics, and Informatics, University of Modena and Reggio Emilia, 41125 Modena, Italy — [2]CNR-Nanoscience Institute, S3 Center, 41125 Modena, Italy

Bottom-up techniques have proven successful to achieve ultra-narrow and structurally well-defined graphene nanoribbons (GNRs) [1-2], where different edge shapes and terminations can be obtained by varying the molecular precursors. In this work we perform density-functional perturbation theory calculations to investigate the vibrational properties of GNRs with cove-type edge structure and variable width, similar to those produced in Ref. 2. By comparison with other prototype systems, we show that the phonon modes and the Raman spectra of these systems strongly depend on the specific edge morphology. This is particularly evident in the acoustic region, where the Radial-Like Breathing Mode (RLBM) shows sensible changes when the edge termination is modified. This makes the Raman spectrum of these GNRs very different from the case of both carbon nanotubes and ribbons with ideal armchair or zigzag edges, where the breathing mode depends on the lateral size only. Our results are in very good agreement with recent experimental data [2].

[1] J. Cai et al., Nature (London) 466, 470 (2010). [2] A. Narita et al., Nature Chem. 6, 126 (2014).

O 16.4 Mon 15:45 ER 164

Controlling the localization of electrons in bilayer graphene — •Maximilian Fleischmann, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle. The small angle regime in particular is associated with significant changes of the electronic properties of the bilayer: one finds localization on the moiré lattice and a significant reduction in the Fermi velocity near the Dirac point [1]. We investigate how the electronic properties in the small angle limit may be controlled by an external electric field directed perpendicular to the bilayer. We consider a uniform field as well as modulated fields with a period chosen to "connect" the Dirac cones of the two layers in momentum space. The latter electrostatic potentials may be realized by a proper choice of substrate. We find that electric fields can be used to control the degree of localization of the quasiparticles in the bilayer. A uniform field tends to delocalize the electron states; this effect is generally less pronounced for energies close to the Dirac point. In contrast, a modulated field favours electron localization throughout the low-energy spectrum.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013.

O 16.5 Mon 16:00 ER 164

Magnetic interactions in bilayer graphene — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The indirect exchange interaction between magnetic impurities, known as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, is governed by the static spin susceptibility of the host system and therefore depends sensitively on the host electronic structure. For this reason, this interaction is particularly interesting for materials in which the underlying electronic spectrum is novel, such as single layer and bilayer graphene. We investigate the RKKY interaction for bilayer graphene at zero and at finite temperature, as well as for the case in which the bilayer is biased by a perpendicular electric field. At the edge of the energy gap between the two conduction (or valence) bands at the Dirac point we find a remarkable transition in the form of the RKKY interaction. For Fermi energies on either side of the gap the interaction takes asymptotically two different forms: the oscillatory or the antiferromagnetic. We show that at the Dirac point the sign of the RKKY interaction (ferromagnetic vs anti-ferromagnetic) can be controlled by an external electric field.

O 16.6 Mon 16:15 ER 164

Is deformed graphene described by the Dirac-Weyl equation on a curved space-time? — •Fabian Rost, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

It is well known that, at low energies, the quasiparticles of graphene are described by the wave equation of massless neutrinos: the Dirac-Weyl equation. Less well understood is whether the elastically deformed graphene can be described as the DW equation on a curved space-time as suggested in [1]. To answer this question we consider both a space-time description, and a low energy treatment derived from the tight-binding model, and compare them term by term in an expansion in the deformation tensor. We find that the low energy theory contains an infinite class of deformation-dependent terms that are absent in the space-time approach. Yet all terms present in the curved-space approach can be found in the low energy theory which follows from the tight-binding model.

[1] F. de Juan, A. Cortijo, and M.A.H. Vozmediano, *P*hys. Rev. B **76**, 165409, 2007.

O 16.7 Mon 16:30 ER 164

Phase diagram of honeycomb lattice in Iionic-Hubbard model — •Sahar Nabavi and Morad Ebrahimkhas — Department of Science, Mahabad Branch, Islamic Azad University, Mahabad 59135, Iran

Tight binding electrons on a honeycomb lattice are described by an effective Dirac theory at low energies. An alternate ionic potential (Δ) generates a single-particle gap in the spectrum. We employ the dynamical mean field theory- iterative perturbation theory (DMFT-IPT) technique, to study the effect of on-site electron correlation (U) on energy gap of a honeycomb system. For a fixed ionic potential Δ, we find that beyond a critical value $U_{c1}(\Delta)$ massive Dirac fermions become massed and we have gapped energy bands. Further increasing U beyond $U_{c2}(\Delta)$, there will be another phase transition to the Mott insulating state. Therefore the competition between the single-particle gap parameter, Δ, and the Hubbard U between $U_{c1}(\Delta) < U < U_{c2}(\Delta)$ restores the semi-metallic nature. The width of the intermediate semi-metallic regime shrinks by increasing the ionic potential. However, at small values of Δ, there is a wide interval of U values for which the system remains semi-metal. The phase diagram and energy gap of the system are identified

O 16.8 Mon 16:45 ER 164

Antiferromagnetic coupling of vacancies in graphene on SiO_2 — •Stephan Zimmermann[1], Sven Just[2], Marco Pratzer[2], Markus Morgenstern[2], Vladislav Kataev[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute of Solid State and Materials Research, 01069 Dresden, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen, Germany

Monolayer graphene grown by chemical vapor deposition and transferred to SiO_2 is used to introduce vacancies by Ar^+ ion bombardment at a kinetic energy of 50 eV. The density of defects visible in scanning tunneling microscopy is considerably lower than the ion fluence, implying that most of the defects are single vacancies as expected from the low ion energy. The vacancies are characterized by scanning tunneling spectroscopy on graphene and highly oriented pyrolytic graphite (HOPG). A peak close to the Dirac point is found within the local density of states of the vacancies similar to the peak found previously for vacancies on HOPG. The peak persists after air exposure up to 180 min, such that electron spin resonance (ESR) at 9.6 GHz can probe the vacancies exhibiting such a peak. After an ion flux of $10/nm^2$, we find an ESR signal corresponding to a g factor of 2.001-2.003 and a spin density of 1-2 spins/nm^2. The peak width is as small as 0.17 mT indicating exchange narrowing. Consistently, the temperature-dependent measurements reveal antiferromagnetic correlations with a Curie-Weiss temperature of -10 K. Thus, the vacancies preferentially couple antiferromagnetically, ruling out a ferromagnetic graphene monolayer at ion induced spin densities of 1-2 nm^2.

O 16.9 Mon 17:00 ER 164

Behaviour of the edge states of the $\nu = 0$ lowest Landau level in graphene beyond SU(4)-symmetry — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris Sud, CNRS, LPTMS, UMR 8626, Orsay 91405 France

The $\nu = 0$ quantum Hall state of an infinite sheet of graphene is known to exhibit various different phases when the SU(4)-symmetry of spin and valley/sublattice isospin is broken by interactions and the Zeeman-effect [1]. The situation becomes even richer when considering the edge states close to the sharp boundaries of a finite piece of graphene: Recent theoretical [2] and experimental [3] works suggest that in finite samples the properties of the spin and isospin-texture and its excitations depend on the position within the lattice with respect to its edge. With the help of numerical Hartree-Fock calculations we theoretically investigate the behaviour of the edge modes of a $\nu = 0$ quantum Hall state of graphene. In our model-Hamiltonian we account for both, the influence of SU(4)-symmetric terms and such that break the symmetry, as well as for the presence of the boundary of the lattice. In doing so, we are able to understand the behaviour of different spin and isospin configurations as compared to the phases in the bulk or the predictions of a non-interacting single-electron theory [4].

[1] M. Kharitonov, Phys. Rev. B **85**, 155439 (2012) [2] G. Murthy *et al.*, Phys. Rev. B **90**, 241410(R) (2014) [3] G. Li *et al.*, Nature Commun. **4**, 1744 (2013) [4] D. A. Abanin *et al.*, Phys. Rev. Lett. **96**, 176803 (2006)